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Bioinformatics Study of Turmeric (*Curcuma domestica Val*) Against Arthritis Gout Disease

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ABSTRACT

Degenerative diseases are developing today. One of them is gouty arthritis, also known as gout. This disease is very common in society. In Indonesia, the prevalence of gouty arthritis is 34-32 years old. According to a report from the Padang City Health Office in 2018, gouty arthritis was ranked the 4th highest disease in the city of Padang after gastritis. The highest prevalence was in North Padang District with 400 sufferers and Alai Health Center ranked 2nd with 118 cases. Gouty arthritis is characterized by high levels of uric acid in the blood (hyperuricemia). Arthritis is rarely fatal, but can be stressful for patients. The therapy used is anti-inflammatory drugs with many side effects. Turmeric (Curcuma longa) is one of the herbal plants that has the potential to treat rheumatism and gout. Turmeric (Curcuma domestica Val) is an herbal plant with anti-inflammatory properties for gouty arthritis. The large old turmeric rhizome is often used as medicine. Turmeric contains the active ingredient curcumin. It has been extensively studied as an anti-inflammatory drug. This is because curcumin can inhibit the protein Cyclooxygenase-2 (COX-2). COX-2 is an enzyme that mediates inflammation. Therefore, the curcumin in turmeric has a potential anti-inflammatory effect and can be used as the basis for the treatment of artritis gout.

Keywords: Artritis gout, *Curcuma domestica Val, Curcumin*

1. INTRODUCTION

Until now, degenerative diseases continue to grow.[1] Degenerative disease is a disease that is often found with age.[2] One of these degenerative diseases is gouty arthritis or better known as gout by the general public. Gouty arthritis is very common in the community.[3] In Indonesia, the prevalence of gout varies. This variation is due to the existing ethnic and cultural diversity.[24][25]

According to a report from the Padang City Health Office in 2018, gouty arthritis was ranked the 4th highest disease in the city of Padang after gastritis. The highest prevalence was in North Padang District with 400 sufferers and Alai Health Center ranked 2nd with 118 cases.[5] The high cases of gouty arthritis are of particular concern, so as not to trigger more serious effects.[26]

Arthritis gout is a disease characterized by high blood uric acid levels (hyperuricemia).[10][11] Arthritis gout is affected by monosodium urate deposition.[12][13] Monosodium urate will form

crystals when uric acid levels in the blood are around 7.0 mgr./dL.[16][17][27][28] In gouty arthritis, monosodium urate crystals trigger an inflammatory process due to the body's response to the formation of monosodium urate crystals.[18][21][22] This inflammatory response can cause joint pain in patients with arthritis gout. This inflammation is characterized by 4 characteristic symptoms: heat, redness, swelling and pain.[23]

Turmeric (Curcuma domestica Val) is an herbal plant with anti-inflammatory properties for arthritis gout.[6] Large old turmeric rhizomes are often used as medicine.

Figure 1. Turmeric Plant

2. LITERATURE REVIEW

Turmeric contains the main active compound, namely curcuminoids.[4][29] Curcuminoids consist of 3 constituents, namely curcumin, demethoxycurcumin, and bisdemethoxycurcumin.[19][20] The curcumin in turmeric has been widely studied for its anti-inflammatory properties.[14][15]

Based on the results of the survey and the theory of problems in patients with gouty arthritis or gout, the authors solve this problem by using computation in exploring the active compounds in the database.[7][30] The author's goal in this case is to maintain uric acid levels in the blood.[8][9]

3. EXPERIMENTAL

This study uses a literature review method or SLR (Systematic Literature Review) approach to review studies, assess and interpret and collect information about the compounds contained in turmeric and its role in treating gout. To find out the content, https://phytochem.nal.usda.gov/ then chemdraw ultra 12.0 and chem 3 D pro 12.0 to make the structure of the compound that already existed at https://pubchem.ncbi.nlm.nih.gov/ previously and define parameters (tables of internal and Cartesian coordinates). In addition, http://swisstargetprediction.ch/ is also used to predict which compound is more active for curing any disease.

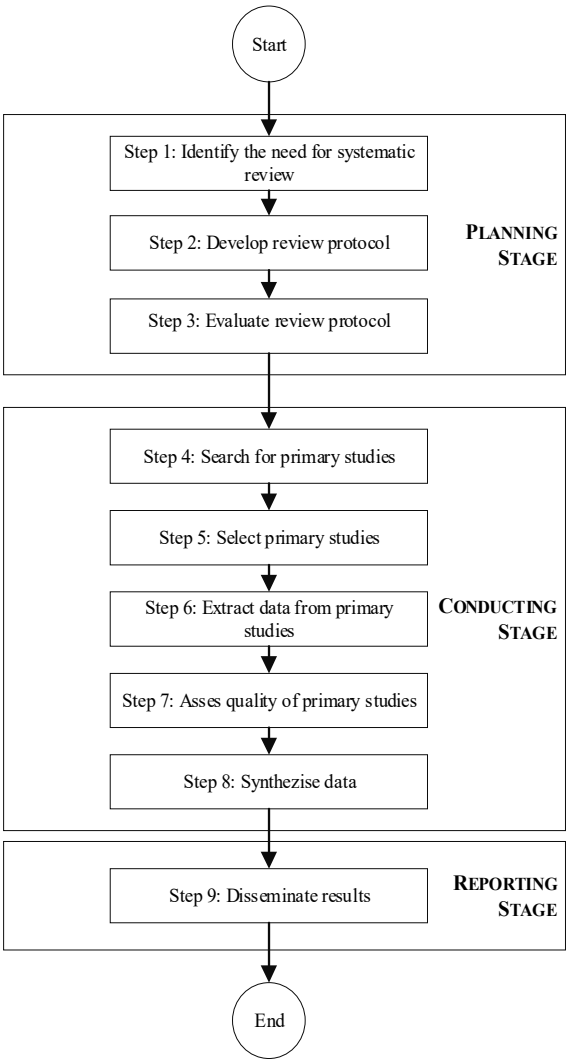

Figure 2. Systematic Review Diagram

Table 1. PICOC Criteria

Population	Naïve Bayes
Intervention	Gout Arthritis
Comparison	-
Outcomes	Solving the problem of gout in the community
Context	Retrospective observational descriptive study

Table 2. Research Question (RQ)

ID	Research Question	Motivation
RQ1	Which journal has published the most research on gout?	Identify journals about gout sufferers.
RQ2	Who is the most active researcher in reporting gout sufferers?	Identifying active researchers in providing data on people with gout.
RQ3	What dataset is most widely used to find out people with gout?	The identification of the most widely used dataset to identify gout sufferers.
RQ4	What methods have been used for previous researchers?	Identify methods that have been carried out by previous researchers about maintaining uric acid levels in the blood.

4. RESULTS AND DISCUSSION

Gout is a disease that occurs due to disorders of purine metabolism, which is characterized by hyperuricemia and acute synovitis. This disease is associated with the accumulation of monosodium monohydrate urate crystals and cartilage degeneration. The incidence of gout is 1-2%, mainly between the ages of 30-40, and the incidence in men is 20 times that in women. Risk factors for gout sufferers include age, excessive intake of purine compounds, excessive alcohol consumption, obesity (overweight), sedentary lifestyle, high blood pressure and heart disease, certain medications (especially diuretics), and kidney damage. Increased levels of uric acid in the blood, in addition to causing gout, according to a study is a strong predictor of death due to cardiovascular damage.

Turmeric contains the main active compound, namely curcuminoids. Curcuminoids consist of 3 constituents, namely curcumin, demethoxycurcumin, and bisdemethoxycurcumin. The curcumin in turmeric has been widely studio for its anti-inflammatory properties.

Various studies have identified several effective ingredients in turmeric which are considered to have good health benefits. The main active ingredient in turmeric is curcuminoids. These curcuminoids give turmeric its color. Curcuminoids consist of 3 components, namely curcumin, demethoxycurcumin and bisdemethoxycurcumin. Gouty arthritis is a chronic disease characterized by inflammation of one or more joints. Treatment of gout attacks is a combination of lifestyle changes and anti-inflammatory drugs, such as the NSAID colchicine, and corticosteroids. However, the use of these anti-inflammatory drugs has a risk of side effects. Long-term use of non-steroidal anti-inflammatory drugs can cause impaired kidney function.

The anti-inflammatory properties of curcumin in turmeric have been studied extensively. A study by Jurenka (2009) showed that curcumin has an anti-inflammatory effect when taken at a dose of 50-200 mg/kg body weight. Research by Muniro et al. (2010) showed that consuming turmeric essential oil at a dose of 25 mg/kg BW for a week could significantly reduce blood urea levels in patients with gouty arthritis.

Besides being easy to obtain and cheap, turmeric also has side effects. In the study of Chandran & Goel (2012), the output of curcumin was safe to use even if it was given long-term for more than 8 weeks. Even in other studies, curcuminoids can suppress the occurrence of kidney toxicity.

Patients with gouty arthritis have deposits of monosodium urate crystals, which can trigger an inflammatory response. Inflammation is characterized by 4 characteristic symptoms: warmth, redness, swelling and pain. This is due to the action of pro-inflammatory cytokines (enzymes that mediate the production of prostaglandins and leukotrienes). The curcumin in turmeric has been widely studied as an anti-inflammatory agent. Curcumin can inhibit the activity of the protein Cyclooxygenase-2 (COX-2). COX-2 acts as an enzyme that mediates prostaglandins. The indirect inhibitory effect of curcumin on COX-2 can inhibit the production of prostaglandins. In addition, turmeric essential oil can reduce levels of TNF-, one of the prostaglandins.

Active compounds in turmeric:
CURCUMIN
IUPAC
(1E,6E)-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione

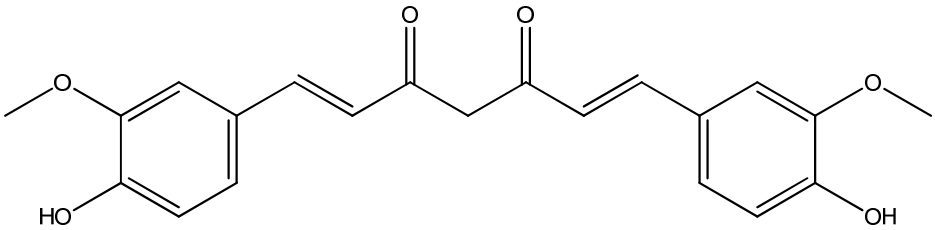

Figure 3. (1E,6E)-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione

Boiling Point: 1065,54 [K]
Melting Point: 761,41 [K]
Critical Temp: 982,7 [K]
Critical Pres: 22,5 [Bar]
Critical Vol: 1035,5 [cm3/mol]
Gibbs Energy: -285,14 [kJ/mol]
Log P: 2,56
MR: 105,79 [cm3/mol]
Henry's Law: 19,54
Heat of Form: -636,43 [kJ/mol]
tPSA: 93.06
CLogP: 2.2506
CMR: 10.615

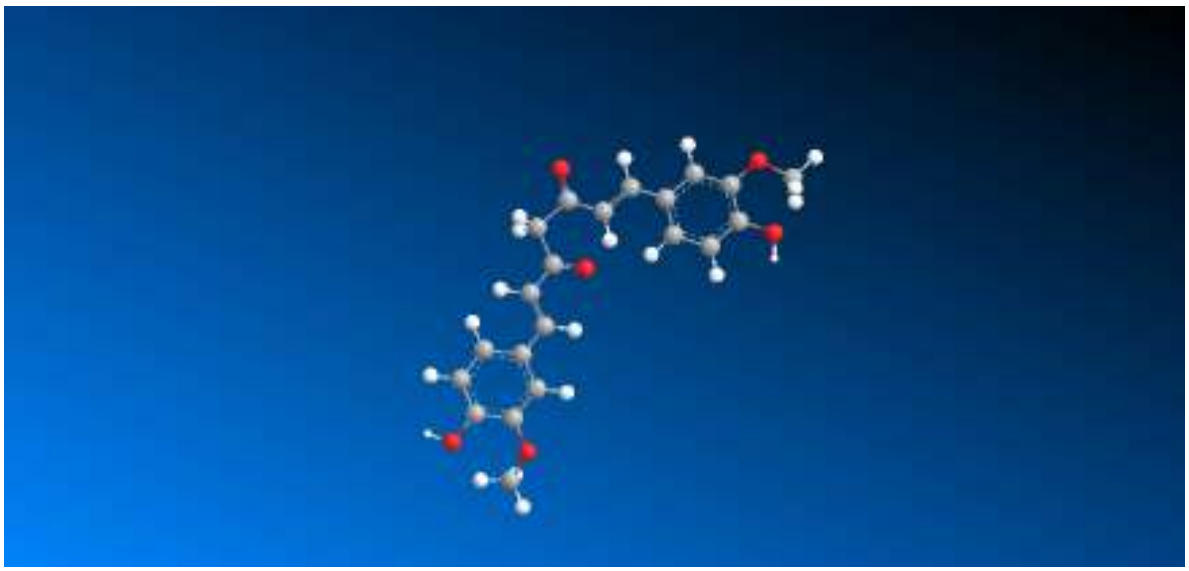

Figure 4. Before optimized

Table 3. Cartesian Table

Atom	X (A)	Y (A)	Z (A)
C(1)	16.995	36.775	-0.8777
C(2)	0.7065	28.120	-0.6486
C(3)	-0.5787	32.140	-0.7576
C(4)	-16.994	22.372	-0.4990
C(5)	-11.209	0.8907	-0.1393
C(6)	-19.426	-0.1459	0.1357
C(7)	-14.301	-13.389	0.4544
O(8)	-0.8306	43.555	-10.622
O(9)	0.0769	0.7396	-0.0972
C(10)	-22.433	-23.647	0.7266
C(11)	-17.086	-36.093	10.591
C(12)	-25.570	-46.795	13.429
C(13)	-39.400	-45.050	12.943
C(14)	-44.747	-32.604	0.9619
C(15)	-36.263	-21.902	0.6780

O(16)	-20.376	-58.886	16.658
C(17)	-26.564	-69.089	0.9297
O(18)	-47.641	-55.446	15.700
C(19)	29.713	32.796	-0.7697
C(20)	40.072	41.825	-10.088
C(21)	53.341	37.674	-0.8963
C(22)	56.250	24.493	-0.5446
C(23)	45.891	15.464	-0.3054
C(24)	32.622	19.616	-0.4180
O(25)	63.404	46.445	-11.286
C(26)	75.877	40.319	-0.9423
O(27)	69.140	20.461	-0.4353
H(28)	14.700	47.169	-11.551
H(29)	0.9360	17.725	-0.3712
H(30)	-23.268	26.076	0.3423
H(31)	-23.248	21.395	-14.145
H(32)	-30.333	-0.0083	0.0974
H(33)	-0.3394	-14.765	0.4928
H(34)	-0.6179	-37.468	10.975
H(35)	-55.654	-31.228	0.9236
H(36)	-40.479	-12.086	0.4158
H(37)	-22.143	-78.907	12.114
H(38)	-37.470	-69.164	11.514
H(39)	-24.991	-67.295	-0.1574
H(40)	-56.806	-52.321	14.853
H(41)	37.777	52.220	-12.861
H(42)	48.186	0.5070	-0.0280
H(43)	24.453	12.495	-0.2295
H(44)	83.972	47.702	-11.383
H(45)	76.671	36.645	0.1053
H(46)	76.888	31.752	-16.455
H(47)	69.146	11.069	-0.1849

Table 4. Internal Coordinates Table

Atom	Bond Atom	Bond Lenght (A	Angel Atom	Angle (º)	2nd Angle Atom	2nd Angle (º)	2nd Angle Type
C(10)							
C(11)	C(10)	13.948					
C(12)	C(11)	13.949	C(10)	1.199.969			
C(13)	C(12)	13.948	C(11)	1.200.002	C(10)	-0.0058	Dihedral
C(14)	C(13)	13.948	C(12)	1.200.033	C(11)	0.0012	Dihedral
C(15)	C(10)	13.948	C(11)	1.200.029	C(12)	0.0058	Dihedral
C(7)	C(10)	13.370	C(11)	1.199.986	C(15)	1.199.986	Pro-R
O(16)	C(12)	13.550	C(11)	1.199.999	C(13)	1.199.999	Pro-R

O(18)	C(13)	13.550	C(12)	1.199.984	C(14)	1.199.984	Pro-R
C(6)	C(7)	13.370	C(10)	1.200.000	C(11)	1.800.000	Dihedral
C(5)	C(6)	13.510	C(7)	1.200.000	C(10)	1.800.000	Dihedral
C(4)	C(5)	15.090	C(6)	1.200.000	C(7)	1.800.000	Dihedral
O(9)	C(5)	12.080	C(4)	1.200.000	C(6)	1.200.000	Pro-S
C(3)	C(4)	15.090	C(5)	1.095.000	C(6)	1.800.000	Dihedral
C(2)	C(3)	13.510	C(4)	1.200.000	C(5)	0.0000	Dihedral
O(8)	C(3)	12.080	C(2)	1.200.000	C(4)	1.200.000	Pro-S
C(1)	C(2)	13.370	C(3)	1.200.000	C(4)	1.800.000	Dihedral
C(19)	C(1)	13.370	C(2)	1.200.000	C(3)	1.800.000	Dihedral
C(20)	C(19)	13.948	C(1)	1.199.986	C(2)	1.800.000	Dihedral
C(24)	C(19)	13.948	C(1)	1.199.986	C(20)	1.200.029	Pro-R
C(21)	C(20)	13.949	C(19)	1.199.969	C(1)	-1.799.942	Dihedral
C(22)	C(21)	13.948	C(20)	1.200.002	C(19)	-0.0058	Dihedral
C(23)	C(24)	13.949	C(19)	1.199.996	C(1)	1.799.988	Dihedral
O(25)	C(21)	13.550	C(20)	1.199.999	C(22)	1.199.999	Pro-S
O(27)	C(22)	13.550	C(21)	1.199.984	C(23)	1.199.984	Pro-S
C(17)	O(16)	14.020	C(12)	1.108.000	C(11)	-1.320.663	Dihedral
C(26)	O(25)	14.020	C(21)	1.108.000	C(20)	1.790.983	Dihedral
H(34)	C(11)	11.000	C(10)	1.200.015	C(12)	1.200.015	Pro-R
H(35)	C(14)	11.000	C(13)	1.200.014	C(15)	1.200.014	Pro-R
H(36)	C(15)	11.000	C(10)	1.200.002	C(14)	1.200.002	Pro-S
H(41)	C(20)	11.000	C(19)	1.200.015	C(21)	1.200.015	Pro-S
H(42)	C(23)	11.000	C(22)	1.200.014	C(24)	1.200.014	Pro-S
H(43)	C(24)	11.000	C(19)	1.200.002	C(23)	1.200.002	Pro-S
H(28)	C(1)	11.000	C(2)	1.200.000	C(19)	1.200.000	Pro-R
H(29)	C(2)	11.000	C(1)	1.200.000	C(3)	1.200.000	Pro-R
H(32)	C(6)	11.000	C(5)	1.200.000	C(7)	1.200.000	Pro-S
H(33)	C(7)	11.000	C(6)	1.200.000	C(10)	1.200.000	Pro-R
H(30)	C(4)	11.130	C(3)	1.094.418	C(5)	1.094.418	Pro-S
H(31)	C(4)	11.130	C(3)	1.094.618	C(5)	1.094.618	Pro-R
H(37)	C(17)	11.130	O(16)	1.095.000	C(12)	1.800.000	Dihedral
H(38)	C(17)	11.130	O(16)	1.094.418	H(37)	1.094.418	Pro-S
H(39)	C(17)	11.130	O(16)	1.094.618	H(37)	1.094.618	Pro-R
H(40)	O(18)	0.9720	C(13)	1.080.000	C(12)	-1.800.000	Dihedral
H(44)	C(26)	11.130	O(25)	1.095.000	C(21)	1.800.000	Dihedral
H(45)	C(26)	11.130	O(25)	1.094.418	H(44)	1.094.418	Pro-S
H(46)	C(26)	11.130	O(25)	1.094.618	H(44)	1.094.618	Pro-R
H(47)	O(27)	0.9720	C(22)	1.080.000	C(21)	-1.800.000	Dihedral

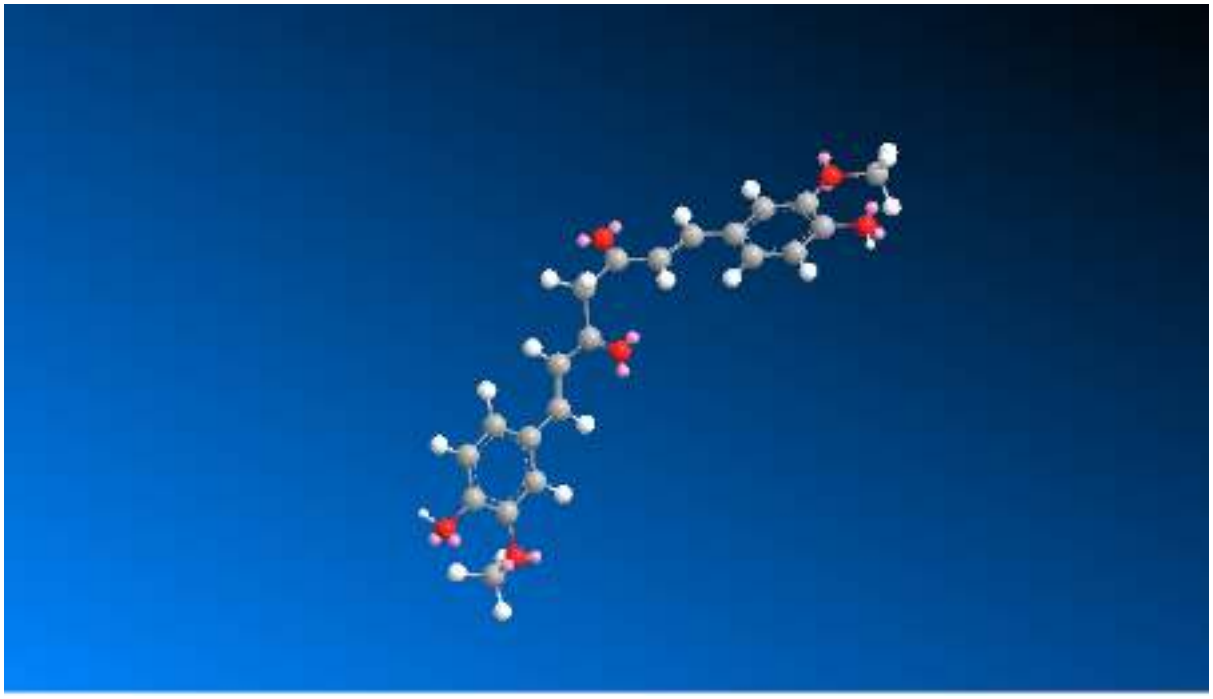

Figure 5. After optimized

----------MM2 Dynamics----------
Pi System: 22 21 8 3 2 1 20 19 23 24
Pi System: 13 12 9 5 6 7 11 10 14 15
Warning: Some parameters are guessed (Quality = 1).

Iteration	Time	Total Energy	Potential Energy	Temperature
5	0.010	262.304 ± 10.599	157.000 ± 19.899	598.78 ± 67.43
10	0.020	275.534 ± 24.183	139.688 ± 16.025	772.44 ±125.80
15	0.030	294.422 ± 9.855	156.411 ± 20.322	784.76 ± 92.49
20	0.040	323.422 ± 58.423	169.028 ± 28.036	877.91 ±341.74
25	0.050	636.925 ± 96.227	399.182 ± 55.012	1351.85 ±641.96

Dynamics terminated because the molecular model is too far from equilibrium
---

----------MM2 Minimization----------
Pi System: 22 21 8 3 2 1 20 19 23 24
Pi System: 13 12 9 5 6 7 11 10 14 15
Warning: Some parameters are guessed (Quality = 1).
Iteration 1800: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch:	2.2488
Bend:	11.5269
Stretch-Bend:	0.1153
Torsion:	-19.3370
Non-1,4 VDW:	1.0171
1,4 VDW:	24.0694
Dipole/Dipole:	1.0443
Total Energy:	20.6849 kcal/mol

Calculation completed

Table 5. Kartesian

Atom	X (A)	Y (A)	Z (A)
C(1)	25.075	40.468	-0.9755
C(2)	13.808	35.086	-0.8334
C(3)	0.0019	36.817	-0.8821
C(4)	-0.6931	22.370	-0.4975
C(5)	-0.4528	0.6450	-0.0786
C(6)	-15.034	-0.1754	0.1457
C(7)	-13.441	-14.749	0.5046
O(8)	-0.7083	47.012	-11.556
O(9)	0.6507	0.2016	0.0440
C(10)	-20.761	-25.784	0.7792
C(11)	-14.636	-37.613	10.693
C(12)	-21.912	-48.522	13.268
C(13)	-35.553	-46.158	13.126
C(14)	-41.120	-34.127	10.452
C(15)	-33.883	-23.566	0.7209
O(16)	-14.146	-59.895	17.015
C(17)	-16.305	-71.830	0.8827
O(18)	-44.359	-55.642	16.672
C(19)	37.566	34.934	-0.8266
C(20)	49.752	40.394	-0.9714
C(21)	62.243	36.107	-0.8548
C(22)	63.636	22.689	-0.4986
C(23)	51.489	16.298	-0.3285
C(24)	39.207	22.029	-0.4818
O(25)	69.841	48.030	-11.661
C(26)	85.011	48.306	-11.548
O(27)	75.941	16.573	-0.3328
H(28)	25.326	51.078	-12.584
H(29)	0.5245	14.025	-0.2782
H(30)	-12.893	25.440	0.3981
H(31)	-12.913	20.605	-14.236
H(32)	-25.745	0.1833	0.0442
H(33)	-0.2754	-17.026	0.5666
H(34)	-0.3530	-37.134	11.136
H(35)	-51.908	-31.703	10.623
H(36)	-38.021	-13.095	0.4857
H(37)	-0.6430	-73.943	0.4753
H(38)	-21.593	-79.879	15.567
H(39)	-21.897	-70.255	-0.0417
H(40)	-52.513	-51.916	20.358
H(41)	48.133	51.037	-12.510
H(42)	50.350	0.5135	-0.0349
H(43)	29.244	13.821	-0.2623

H(44)	84.557	59.051	-13.977
H(45)	89.456	46.244	-0.1342
H(46)	89.690	41.962	-19.797
H(47)	74.493	0.7281	-0.0670

Table 6. Internal Coordinates

Atom	Bond Atom	Bond Lenght (A	Angel Atom	Angle (°)	2nd Angle Atom	2nd Angle (°)	2nd Angle Type
C(10)							
C(11)	C(10)	13.948					
C(12)	C(11)	13.949	C(10)	1.199.969			
C(13)	C(12)	13.948	C(11)	1.200.002	C(10)	-0.0058	Dihedral
C(15)	C(10)	13.948	C(11)	1.200.029	C(12)	0.0058	Dihedral
H(34)	C(11)	11.000	C(10)	1.200.015	C(12)	1.200.015	Pro-R
C(7)	C(10)	13.370	C(11)	1.199.986	C(15)	1.199.986	Pro-R
C(14)	C(13)	13.948	C(12)	1.200.033	C(11)	0.0012	Dihedral
O(16)	C(12)	13.550	C(11)	1.199.999	C(13)	1.199.999	Pro-R
C(6)	C(7)	13.370	C(10)	1.200.000	C(11)	1.800.000	Dihedral
C(17)	O(16)	14.020	C(12)	1.108.000	C(11)	-1.320.663	Dihedral
O(18)	C(13)	13.550	C(12)	1.199.984	C(14)	1.199.984	Pro-R
H(35)	C(14)	11.000	C(13)	1.200.014	C(15)	1.200.014	Pro-R
H(36)	C(15)	11.000	C(10)	1.200.002	C(14)	1.200.002	Pro-S
Lp(52)	O(16)	0.6000	C(12)	1.091.162	C(17)	1.091.162	Pro-S
Lp(53)	O(16)	0.6000	C(12)	1.087.026	C(17)	1.087.026	Pro-R
C(5)	C(6)	13.510	C(7)	1.200.000	C(10)	1.800.000	Dihedral
H(33)	C(7)	11.000	C(6)	1.200.000	C(10)	1.200.000	Pro-R
H(37)	C(17)	11.130	O(16)	1.095.000	C(12)	1.800.000	Dihedral
H(40)	O(18)	0.9720	C(13)	1.080.000	C(12)	-1.800.000	Dihedral
Lp(54)	O(18)	0.6000	C(13)	1.098.151	H(40)	1.098.151	Pro-S
Lp(55)	O(18)	0.6000	C(13)	1.103.348	H(40)	1.103.348	Pro-R
C(4)	C(5)	15.090	C(6)	1.200.000	C(7)	1.800.000	Dihedral
H(32)	C(6)	11.000	C(5)	1.200.000	C(7)	1.200.000	Pro-S
H(38)	C(17)	11.130	O(16)	1.094.418	H(37)	1.094.418	Pro-S
H(39)	C(17)	11.130	O(16)	1.094.618	H(37)	1.094.618	Pro-R
C(3)	C(4)	15.090	C(5)	1.095.000	C(6)	1.800.000	Dihedral
O(9)	C(5)	12.080	C(4)	1.200.000	C(6)	1.200.000	Pro-S
C(2)	C(3)	13.510	C(4)	1.200.000	C(5)	0.0000	Dihedral
H(30)	C(4)	11.130	C(3)	1.094.418	C(5)	1.094.418	Pro-S
H(31)	C(4)	11.130	C(3)	1.094.618	C(5)	1.094.618	Pro-R
Lp(50)	O(9)	0.6000	C(5)	1.200.000	C(4)	-1.800.000	Dihedral
Lp(51)	O(9)	0.6000	C(5)	1.090.000	C(4)	0.0000	Dihedral
C(1)	C(2)	13.370	C(3)	1.200.000	C(4)	1.800.000	Dihedral
O(8)	C(3)	12.080	C(2)	1.200.000	C(4)	1.200.000	Pro-S

C(19)	C(1)	13.370	C(2)	1.200.000	C(3)	1.800.000	Dihedral
H(29)	C(2)	11.000	C(1)	1.200.000	C(3)	1.200.000	Pro-R
Lp(48)	O(8)	0.6000	C(3)	1.200.000	C(2)	-1.800.000	Dihedral
Lp(49)	O(8)	0.6000	C(3)	1.090.000	C(2)	0.0000	Dihedral
C(20)	C(19)	13.948	C(1)	1.199.986	C(2)	1.800.000	Dihedral
H(28)	C(1)	11.000	C(2)	1.200.000	C(19)	1.200.000	Pro-R
C(21)	C(20)	13.949	C(19)	1.199.969	C(1)	-1.799.942	Dihedral
C(24)	C(19)	13.948	C(1)	1.199.986	C(20)	1.200.029	Pro-R
C(22)	C(21)	13.948	C(20)	1.200.002	C(19)	-0.0058	Dihedral
C(23)	C(24)	13.949	C(19)	1.199.996	C(1)	1.799.988	Dihedral
H(41)	C(20)	11.000	C(19)	1.200.015	C(21)	1.200.015	Pro-S

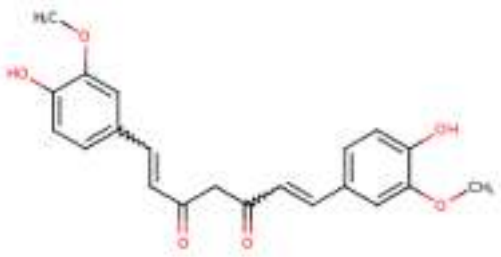

Figure 6. Structure Prediction

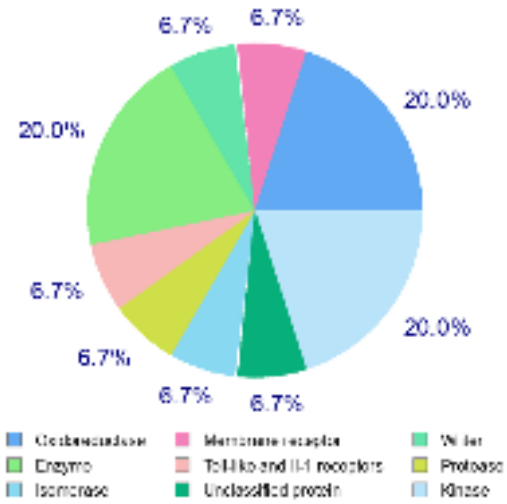

Figure 7. Structure Prediction

5. CONCLUSION

Turmeric (Curcuma domestica Val.) is a well-known plant. This plant is easy to get and cheap. Turmeric has health benefits, one of which is anti-inflammatory. When compared with drug therapy that has a risk of side effects, turmeric therapy can be an alternative method, but further research is needed to be effective and efficient.

Based on the descriptive results and data analysis on turmeric, three active compounds were obtained, namely curcumin, demethoxycurcumin, and bisdemethoxycurcumin. Where in curcumin contains 20.0% oxidoreductse, 20.0% enzyme, 6.7% isomerase, 6.7% membrane receptor, 6.7% toll-like and il-1 receptors, 6.7% unclassified protein, 6.7% writer, 6.7 protease and 20.0% kinase. Demethoxycurcumin contains 6.7% protease, 6.7% writer, 6.7% membrane receptors, 6.7% surface antigen, 13.3% oxidoreductase, 26.7% enzyme, 6.7% isomerase, 6.7% toll-like and il-1 receptors and 20.0% kinase. Bisdemethoxycurcumin contains 20.0% protease, 6.7% writer, 6.7% isomerase, 20.0% oxidoreductase, 20.0% enzyme, 6.7% unclassified protein, 6.7% membrane receptor, 6.7% toll-like and ill-1 receptors and 20.0% kinase.

REFERENCES

[1] Holan, V., Palacka, K., & Hermankova, B. (2021). Mesenchymal stem cell-based therapy for retinal degenerative diseases: experimental models and clinical trials. *Cells*, *10*(3), 588.

[2] Calabrese, E. J., & Kozumbo, W. J. (2021). The phytoprotective agent sulforaphane prevents inflammatory degenerative diseases and age-related pathologies via Nrf2-mediated hormesis. *Pharmacological Research*, *163*, 105283.

[3] Patil, T., Soni, A., & Acharya, S. (2021). A brief review on in vivo models for Gouty Arthritis. *Metabolism Open*, *11*, 100100.

[4] Afifah, D., Arief, M., & Al-Arif, M. A. (2021, February). The effect of garlic (Allium sativum) and turmeric (Curcuma longa) extract addition in commercial feed on feeding rate, feed efficiency and feed conversion ratio of gouramy fish (Osphronemus gouramy). In *IOP Conference Series: Earth and Environmental Science* (Vol. 679, No. 1, p. 012073). IOP Publishing.

[5] Berger, M., Bastl, M., Bouchal, J., Dirr, L., & Berger, U. (2021). The influence of air pollution on pollen allergy sufferers. *Allergologie Select*, *5*, 345.

[6] Fatimah, S., Syafrini, D., & Zainul, R. (2021). Rendang lokan: history, symbol of cultural identity, and food adaptation of Minangkabau tribe in West Sumatra, Indonesia. *Journal of Ethnic Foods*, *8*(1), 1-10.

[7] Febriani, S. S., Yolanda, T., Arianti, V. A., & Zainul, R. (2018). A Review Solid Stated: Principles and Methode.

[8] Russo, E., Viazzi, F., Pontremoli, R., Barbagallo, C. M., Bombelli, M., Casiglia, E., ... & Borghi, C. (2021). Association of uric acid with kidney function and albuminuria: the Uric Acid Right for heArt Health (URRAH) Project. *Journal of Nephrology*, 1-11.

[9] Zainul, R., Hashim, N., Yazid, S. N. A. M., Sharif, S. N. M., Ahmad, M. S., Saidin, M. I., ... & Isa, I. M. (2021). Magnesium layered hydroxide-3-(4-methoxyphenyl) propionate modified single-walled carbon nanotubes as sensor for simultaneous determination of Bisphenol A and Uric Acid. *International Journal of ELECTROCHEMICAL SCIENCE*, *16*, 1-11.

[10] Topless, R. K., Phipps-Green, A., Leask, M., Dalbeth, N., Stamp, L. K., Robinson, P. C., & Merriman, T. R. (2021). Gout, rheumatoid arthritis, and the risk of death related to coronavirus disease 2019: an analysis of the UK biobank. *ACR Open Rheumatology*, *3*(5), 333-340.

[11] Nurashikin, A. A., Isa, I. M., Hashim, N., Ahmad, M. S., Siti, N. A. M. Y., Saidin, M. I., ... & Mukdasai, S. (2019). Voltammetric Determination of Bisphenol A in the Presence of Uric Acid Using a Zn/Al-LDH-QM Modified MWCNT Paste Electrode. *International Journal of ELECTROCHEMICAL SCIENCE*, *14*.

[12] Sun, L., Yuan, G., Gao, L., Yang, J., Chhowalla, M., Gharahcheshmeh, M. H., ... & Liu, Z. (2021). Chemical vapour deposition. *Nature Reviews Methods Primers*, *1*(1), 1-20.

[13] Dinata, A. A., Rosyadi, A. M., Hamid, S., & Zainul, R. (2018). A Review Chemical Vapor Deposition: Process And Application.

[14] Fiorito, S., Epifano, F., Preziuso, F., Palumbo, L., Marchetti, L., Bastianini, M., ... & Genovese, S. (2021). Solid-Phase Adsorption of Curcumin from Turmeric Extracts by Lamellar Solids and Magnesium Oxide and Hydroxide. *Food Analytical Methods*, *14*(6), 1133-1139.

[15] Candani, D., Ulfah, M., Noviana, W., & Zainul, R. (2018). A Review Pemanfaatan Teknologi Sonikasi.

[16] Cipolletta, E., Di Battista, J., Di Carlo, M., Di Matteo, A., Salaffi, F., Grassi, W., & Filippucci, E. (2021). Sonographic estimation of monosodium urate burden predicts the fulfillment of the 2016 remission criteria for gout: a 12-month study. *Arthritis Research & Therapy*, *23*(1), 1-10.

[17] Kristy, D. P., & Zainul, R. (2019). Analisis Molekular dan Transpor Ion Natrium Silikat.

[18] Han, J., Shi, G., Li, W., Xie, Y., Li, F., & Jiang, D. (2021). Preventive effect of dioscin against monosodium urate-mediated gouty arthritis through inhibiting inflammasome NLRP3 and TLR4/NF-κB signaling pathway activation: an in vivo and in vitro study. *Journal of natural medicines*, *75*(1), 37-47.

[19] Nuamsee, K., Chuprajob, T., Pabuprapap, W., Jintaridth, P., Munkongdee, T., Phannasil, P., ... & Svasti, S. (2021). Trienone analogs of curcuminoids induce fetal hemoglobin synthesis via demethylation at Gγ-globin gene promoter. *Scientific reports*, *11*(1), 1-9.

[20] Firdaus, A., & Zainul, R. (2018). SESIUM KLORIDA (CsCl): TRANSPORT ION DALAM LARUTAN.

[21] Lauterbach, M. A., Saavedra, V., Mangan, M. S., Penno, A., Thiele, C., Latz, E., & Kuerschner, L. (2021). 1-Deoxysphingolipids cause autophagosome and lysosome accumulation and trigger NLRP3 inflammasome activation. *Autophagy*, *17*(8), 1947-1961.

[22] Djasli, Y. A., Purnamasari, D., & Zainul, R. (2020, March). Study of dynamically catalytic system on humic acid phototranformator. In *Journal of Physics: Conference Series* (Vol. 1481, No. 1, p. 012037). IOP Publishing.

[23] Qu, G., Chen, J., Huang, G., Zhang, M., Yu, H., Zhu, H., ... & Pei, B. (2021). A quantitative exploration of symptoms in COVID-19 patients: an observational cohort study. *International journal of medical sciences*, *18*(4), 1082.

[24] Kauh, T. J., Read, J. N. G., & Scheitler, A. J. (2021). The critical role of racial/ethnic data disaggregation for health equity. *Population research and policy review*, *40*(1), 1-7.

[25] Anhar, A., Sumarmin, R., & Zainul, R. (2016). Measurement of glycemic index of West Sumatera local rice genotypes for healthy food selection. *Journal of Chemical and Pharmaceutical Research*, *8*(8), 1035-1040.

[26] Xie, X., Zou, J., Fontes-Garfias, C. R., Xia, H., Swanson, K. A., Cutler, M., ... & Shi, P. Y. (2021). Neutralization of N501Y mutant SARS-CoV-2 by BNT162b2 vaccine-elicited sera. *BioRxiv*.

[27] Kawasoe, S., Kubozono, T., Ojima, S., Kawabata, T., Miyahara, H., Tokushige, K., & Ohishi, M. (2021). J-shaped curve for the association between serum uric acid levels and the prevalence of blood pressure abnormalities. *Hypertension Research*, *44*(9), 1186-1193.

[28] Zainul, R., Hashim, N., Yazid, S. N. A. M., Sharif, S. N. M., Ahmad, M. S., Saidin, M. I., ... & Isa, I. M. (2021). Magnesium layered hydroxide-3-(4-methoxyphenyl) propionate modified single-walled carbon nanotubes as sensor for simultaneous determination of Bisphenol A and Uric Acid. *International Journal of ELECTROCHEMICAL SCIENCE*, *16*, 1-11.

[29] Patil, S. S., Pathak, A., & Rathod, V. K. (2021). Optimization and kinetic study of ultrasound assisted deep eutectic solvent based extraction: A greener route for extraction of curcuminoids from Curcuma longa. *Ultrasonics sonochemistry*, *70*, 105267.

[30] Kulli, V. R., & Gutman, I. (2021). Computation of Sombor indices of certain networks. *SSRG International Journal of Applied Chemistry*, *8*(1), 1-5.