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Original Research Article

Identification, Characterization and *In-Silico* Study of Anti-Ulcer Phytoconstituents of Unripe *Musa Sapien*tum Fruits

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ABSTRACT

There have been age long practices among different traditions and cultures about the use of traditional remedies for prevention and treatment of diseases which had been handed down to generations. In order to make these remedies acceptable to modern medicine, there is a need to scientifically evaluate, identify the active principles and understand their mechanism of action. Unripe *Musa sapientum* fruit was purchased from Ijesha local market in Ogun State, identified and authenticated with authentication number LUH: 100777. The fruits were processed, sliced, dried, pulverized and extracted by cold maceration. Crude extract was fractionated by liquid-liquid partitioning. Identification of the phytoconstituents was carried out by two powerful analytical techniques: Gas Chromatography-Mass Spectrometry (GC-MS) and High-Performance Liquid Chromatography-Mass Spectrometry (HPLC-MS). *In silico* study was carried out on the identified components using Schrodinger Maestro 12.8 Suite 2021–2, two receptors were employed as proteins: 6M9T and 5YLU; two standard anti-ulcer drugs were employed. Results showed that GC-MS identified and characterized fragments components of the phytoconstituents while HPLC-MS identified and quantified the actual phytoconstituents. Molecular docking proved that some fragments had higher affinity and greater interaction than the standard drugs at 5YLU receptor while misoprostol showed higher affinity and greater interaction than fragment, but quercetin showed greater affinity proved by higher docking score at 6M9T receptor. Some identified compounds had anti-ulcer potentials as indicated by their docking scores. These components could be integrated into drug discovery pipeline, they might form LEAD and HIT for a new or novel anti-ulcer drug discovery and development.

Keywords: Identification, Phytoconstituents, Molecular docking, Receptor interaction, *Musa sapientm.*

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Introduction

Natural products have been an integral part of the ancient traditional medicine system. According to the world health organization (WHO), a medicinal plant is any plant which contains substances that can be used for therapeutic purpose [1]. The mechanism of action of most herbal medicines has not been fully understood, and experience obtained from their traditional use over the years should not be ignored [2]. In order to make these remedies acceptable to modern medicine, there is a need to scientifically evaluate, identify the active principles and understand the mechanism of action [2].

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The process of passing down knowledge on the use of traditional medicine for the treatment of diseases from generation to generation in various parts of the world, has significantly contributed to the development of different traditional systems of medicine as well as helped in exploration of different medicinal plants to find the scientific basis of their traditional uses[3]. Exploration of biologically active natural products have played a pivotal role in discovering new chemical entities[3], for example, approximately 28% of NCEs between 1981 and 2002 were natural products or natural product-derived. About 40% of prescription drugs are derived from herbs and about half of the world's best-selling pharmaceutical preparations are derivatives of natural products [4].

Peptic ulcer disease (PUD) is a combination of diverse disorder which is evident as erosion or sore on the gastrointestinal mucosa lining [5]. *Helicobacter pylori*-associated PUD and NSAID-associated PUD account for the majority of the disease etiology [6,7]. An imbalance between aggressive factors and the maintenance of mucosal integrity via endogenous defense mechanisms is believed to be the etiology of the disease[5,8,9,10,11,12]. *H. pylori* accounts for 90% of duodenal ulcers and 70 to 90% of gastric ulcers [5,6]. *Musa sapientum* had been shown to possess phytochemical compounds which produce promising results in the treatment gastrointestinal disorders such as peptic ulcer disease [PUD] [13,14]. The search for an ideal anti-ulcer drug continues and has also been extended to herbal and medicinal plants. Bioactive molecules (generally alkaloids, glycosides, lupeols, essential oils, e.t.c) isolated from crude extracts have been used directly as therapeutic agents or as starting materials for the synthesis of useful

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drugs or serve as a model for pharmacologically active compounds in the process of drug synthesis[14].
This study aimed to identify, characterize and quantify the phytochemical compounds responsible for the anti-ulcer potential of unripe *Musa sapientum* fruits and carry out an *in-silico* study on the identified phytoconstituents to ascertain the relationship between them and the receptors implicated in ulceration.

Materials and Methods

Collection and Identification of Plant Materials
Unripe *Musa sapientum* fruit was purchased in May, 2025 from Ijesha local market in Ogun State, identified and authenticated with authentication number LUH: 100777. The fruits were processed, sliced, dried at room temperature, pulverized and extracted by cold maceration in the ratio of 1;2 ($^{w}/_{v}$) using 80% ethanol. The extract was concentrated in Stuart rotary evaporator set at 40°C and 72RPM and then dried in hot air oven set at 40°C.
Crude extract was fractionated by liquid-liquid partitioning using four different solvents: n-Hexane, Chloroform, Ethyl acetate and n-Butanol. Thirty grams of the CE was weighed and reconstituted in distil water at the ratio of 1:8 ($^{w}/_{v}$) and was shaken vigorously. An equal volume of n-Hexane was added into the homogenous mixture and was agitated for five minutes in a separating funnel. The mixture was allowed to stand for 30minutes. Then, n-Hexane fraction was separated and the same procedure was carried out on other solvents: (n-Hexane, Chloroform, Ethyl acetate and n-Butanol). The fractions were concentrated in rotary evaporator, labelled as FB, FC, FE and FH, dried in a hot air oven set at 40°C and stored in a refrigerator.
Identification of the phytochemical constituents was carried out by two powerful analytical techniques: Gas Chromatography-Mass Spectrometry (GC-MS) and High-Performance Liquid Chromatography-Mass Spectrometry (HPLC-MS). The working condition of GC-MS was set as follows: Machine: Agilent 5977D GC/MSD system coupled with Agilent 8860 auto – sampler; ionization energy of 70 eV; carrier gas: Helium (99.999%) with constant flow rate of 1ml/min; injection volume: 1µl; split ratio: 10:1. The injection temperature was maintained at 300°C, the ion source temperature was 250°C, and the oven temperature was programmed from 100°C (Isothermal for 0.5min), with an increase of 10°C/min to 280°C (2.5min), mass spectra was taken at 70 eV; a scanning interval of 0.5s and fragments of 45 to 450 Da. The solvent delay was 0 to 10mins at 28min/run. The high separation power of GC is complemented by the identification capabilities of the MS. HPLC-MS combines the separation capabilities of HPLC with the mass analysis capabilities of mass spectrometry and the working condition was set as follows: Model: Agilent 1260LC, Mobile Phase: ACN:0.1% Formic Acid (80:20), Column: Poroshell C18, (30x2.1mm), DAD:(VWD): 257nm, Flow Rate 0.700mL/min, Temperature: 28°C, Wavelength: 257. Quercetin was used to calibrate the machine and thus regarded as the standard. HPLC-MS separate, identify, and provide amount per area of the components within a mixture. GC-MS separated, identified and characterized the phytoconstituents of the crude extract while HLC-MS separated, identified, quantified the phytoconstituents of the crude extracts and fractions. Data obtained were analysed by ANOVA, followed by Dunnett's multiple comparison test using Graph-Pad PRISM 8 software. P-values <0.05 were considered as significant.

Molecular Docking
In silico study was carried out on the identified phytochemical components using Schrodinger Maestro 12.8 Suite 2021–2. Two receptors implicated in ulceration were identified from Protein Data Base (PDB) as 6M9T and 5YLU (PGE and H^{+}/K^{+}ATPase respectively), their structures were prepared with the Schrodinger program. Prime was used to add any missing side chains and loops. The structure was optimized (protonation) with OPLS4 and minimized with PROPKA after water molecules above 5.00 of the heteroatoms were eliminated. Then, the ligand-binding pocket was defined using the receptor grid file (5YLU COORDINATES: 49.3; -15.7 and -3.18 as X, Y and Z; 6M9T COORDINATES: 129.3; -7.36 and 154.5 as X, Y and Z)**.** 2D and 3D structures of the identified phytochemicals were downloaded from PUBCHEM data base repository with right chiralities, 2D and 3D structures of two standard anti-ulcer drugs were also downloaded and prepared as ligands. They were neutralized (to remove all ions after crystallization), Desalted, tautomers generated and ligprep was then generated. By creating a receptor grid for ligand docking, it was possible to establish the location and dimensions of the protein's active region. The generated receptor grid file was used to conduct molecular docking research using the Glide tool in Schrodinger Maestro 12.8. High Throughput Virtual Screening (HTVS) was first used to ensure precision, faster and accuracy of the scores, followed by Standard Precision (SP), and finally Extra precision (XP).

Results and Discussion

The result obtained from extraction revealed that 1000g of material extracted in 2000ml solvent yielded 58.9g of crude extract which is approximately 5.9% yield. Results of fractionation revealed ethyl acetate with the highest yield suggesting that those phytoconstituents might be more soluble in the solvent than others. Table 1 revealed the results of the fractionation yields.

Table 1: Fractionation

Fractions	Yields (g)	Percentage yields (%)
n-Hexane	1.6	5.33
Chloroform	0.4	1.33
Ethyl acetate	17	56.67
n-Butanol	0.9	3
Residue (H_2O soluble)	4.8	16

The results obtained from the characterization of crude extract of *Musa sapientum* showed that the fruit contained a lot of phytoconstituents namely: silane, silanol, pentaborane, propane, formamide, methanamine, 1-eicosanol, L-sorbose, cyclohexane, thiazolidine, 6-tridecane, Formamide, Methanamine, 1-Azabicyclo[2.2.2]octan-3-one, 1-Eicosanol, etc. Result of GC-MS characterization of crude extract was tabulated in Table 2.
Identification and quantification analysis carried out on the crude extract and different fractions of *Musa sapientum* showed that the fruit possessed different phytochemicals including phenolic compounds, e.gs. caffeic acid, ferulic acid, maleic acid, gallic acid, salicylic acid, tannic acid, saponins, and poly phenolic compounds e.gs. apigenin, rutin hydrate, naringenin, kaempferol, quercetin and p-coumaric acid. Tables 3a, 3b, 3c, 3d and 3e revealed the phytoconstituents of *Musa sapientum* fruit of crude extract (CE), n-Butanol (FB), Chloroform (CE), Ethyl acetate (FC), and n-Hexane (FH) fractions respectively. Results obtained from the molecular docking were tabulated in Tables 4a, 4b, 4c and 4d**.** The higher the negativity, the greater affinity and better interactions with the receptors.

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Table 2: Phytoconstituents of Characterization

Compound number (#)	RT (min)	Scan number (#)	Area (Ab*s)	Baseline Heigtht (Ab)	Absolute Heigtht (Ab)	Peak Width 50% (min)	Hit Number	Hit Name	Quality	Mol Weight (amu)	CAS Number	% Composition
1	3.161	13	74486	51391	53940	0.057	1	Silane, methylenebis-	9	76.016	001759-88-2	2.58
2	3.413	57	74010	47192	52451	0.074	1	Silanol, dimethyl-	9	76.034	005906-76-3	2.56
3	3.962	153	21986	11514	15097	0.057	1	Pentaborane(9)	50	64.117	019624-22-7	0.76
4	4.105	178	33006	21517	26228	0.069	1	Propane, 1-(ethylthio)-2-methyl-	9	118.082	001613-45-2	1.14
5	4.912	319	25619	15000	18088	0.057	1	Formamide, N-methylthio	5	75.014	018952-41-5	0.89
6	5.084	349	74626	45666	65700	0.063	1	Methanamine, N-methoxy-	9	61.053	001117-97-1	2.58
7	5.187	367	53899	36605	58759	0.057	1	Methanamine, N-methoxy-	9	61.053	001117-97-1	1.86
8	8.54	953	42460	16014	17905	0.114	1	1-Azabicyclo[2.2.2]octan-3-one	25	125.084	003731-38-2	1.47
9	11.235	1424	58201	21793	22786	0.109	1	1-(2-Hydroxyethylthio)-2-(2-vinylthioethoxy)ethane	17	208.059	114811-41-5	2.01
10	12.642	1670	93490	33594	39454	0.143	1	Methyl-3,4-O-furylidene.beta.l-arabinopyranoside	32	242.079	053547-58-3	3.23
11	13.135	1756	79900	16470	22697	0.143	1	1-Eicosanol	37	298.324	000629-96-9	2.76
12	13.793	1871	547059	93407	137615	0.172	1	L-Sorbose	47	180.063	000087-79-6	18.93
13	17.031	2437	323417	130379	132003	0.149	1	n-Hexadecanoic acid	91	256.24	000057-10-3	11.19
14	17.352	2493	437300	217426	219530	0.103	1	Hexadecanoic acid, ethyl ester	90	284.272	000628-97-7	15.13
15	18.616	2714	163394	70789	71822	0.109	1	Cyclohexane, methylene-	81	96.094	001192-37-6	5.65
16	18.668	2723	202543	66324	69377	0.177	1	3-Tetradecen-5-yne, (E)-	47	192.188	074744-44-8	7.01
17	18.885	2761	304805	149229	152765	0.086	1	6-Tridecane	89	180.188	042371-66-4	10.54
18	18.942	2771	135146	77026	100365	0.057	1	4,7-Methano-2H-inden-2-one, octahydro-	50	150.104	050447-20-6	4.68
19	19.171	2811	51880	26483	29229	0.08	1	Thiazolidine, 2-ethyl-	35	117.061	024050-09-7	1.79
20	23.056	3490	93359	35643	49770	0.086	1	2-Oxatricyclo[4.3.1.0(3,8)]decan-10-one	59	152.084	1000187-01-6	3.23
			2890586									100.00

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Table 3a: Phytoconstituents of CE

Name	Ret.time (min)	Area (mAU*s)	Amt/area ± SEM
Quercetin	12.432	3.946	3.400 ± 0.00088
Caffeic acid	1.392	0.347	0.6300 ± 0.0035
Ferulic acid	1.568	57.42	0.03867 ± 0.0034
Maleic acid	2.270	14.35	0.09633 ± 0.0015
Gallic acid	3.091	76.67	0.01933 ± 0.00145
Salicylic acid	3.567	4.643	0.2977 ± 0.00088
Tannic acid	4.468	6.395	0.06867 ± 0.0018
Apigenin	5.126	3.152	0.2240 ± 0.00252
Rutin hydrate	6.026	2.157	0.2913 ± 0.0012
Naringin	7.125	3.559	0.2270 ± 0.00116
Kaempferol	10.194	1.523	0.4513 ± 0.0119
p-Coumaric acid	14.236	0.838	3.400 ± 0.00088

Table 3b: Phytoconstituents of FB

Name	Ret.time (min)	Area (mAU*s)	Amt/area ± SEM
Quercetin	12.453	0.024	1.599 ± 0.000577
Caffeic acid	1.348	582.8	0.6323 ± 0.00088
Ferulic acid	1.607	211.7	0.04133 ± 0.00145
Maleic acid	2.294	404.2	0.09600± 0.00058
Gallic acid	3.090	0.000	0.000
Salicylic acid	3.580	0.000	0.000
Tannic acid	4.407	1.065	0.06533 ± 0.0012
Apigenin	5.394	0.028	0.2237 ± 0.00285
Rutin hydrate	6.148	0.052	0.2910 ± 0.00153
Naringin	7.008	1.052	0.2277 ± 0.00176
Kaempferol	10.215	0.202	0.4550 ± 0.00351
p-Coumaric acid	14.028	0.026	3.404 ± 0.00285

Table 3c: Phytoconstituents of FC

Name	Ret.time (min)	Area (mAU*s)	Amt/area ± SEM
Quercetin	7.949	0.035	0.00735 ± 0.00012
Caffeic acid	1.275	3.571	0.00050 ± 0.00022
Ferulic acid	1.490	0.000	0.000
Maleic acid	1.514	0.000	0.000
Gallic acid	1.982	0.076	0.00233 ± 0.00018
Salicylic acid	2.615	0.383	0.00080 ± 3.651e-005
Tannic acid	3.352	0.000	0.000
Rutin hydrate	6.407	0.169	0.00558 ± 9.458e-005
Kaempferol	6.874	0.062	0.000983 ±4.773e-005
Naringin	7.949	0.013	0.00180 ± 8.563e-005
p-Coumaric acid	11.316	0.877	0.00698 ± 7.032e-005

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Table 3d: Phytoconstituents of FE

Name	Ret.time (min)	Area (mAU*s)	Amt/area ± SEM
Quercetin	7.899	3.335	0.007467 ±0.00012
Caffeic acid	1.272	3.382	0.0004333±0.000285
Ferulic acid	1.499	12.169	0.006900 ±5.774e-005
Maleic acid	1.519	0.000	0.000
Gallic acid	1.979	0.226	0.002567 ±0.00022
Salicylic acid	2.541	170.045	0.0007667 ± 3.3e-005
Tannic acid	3.385	0.104	0.0004667 ± 3.3e-005
Rutin hydrate	6.376	1.276	0.0055 ± 5.774e-005
Kaempferol	6.961	1.420	0.00093 ± 3.333e-005
p-Coumaric acid	11.287	0.036	0.00680 ± 5.774e-005

Table 3e: Phytoconstituents of FH

Name	Ret.time (min)	Area (mAU*s)	Amt/area ± SEM
Quercetin	7.945	55.464	0.00747 ±0.0001202
Caffeic acid	1.276	1.472	0.00013 ± 3.333e-005
Ferulic acid	1.490	0.000	0.000
Maleic acid	1.609	5035.1	0.00237 ± 3.333e-005
Gallic acid	1.850	1.694	0.00240 ± 5.774e-005
Salicylic acid	2.570	0.000	0.000
Tannic acid	3.410	7.227	0.000467 ±3.333e-005
Rutin hydrate	6.353	0.079	0.00550 ± 5.774e-005
Kaempferol	6.964	164.96	0.00933 ±8.819e-005
Naringin	7.361	110.181	0.00170 ± 5.774e-005
p-Coumaric acid	11.291	0.073	0.006933 ±8.819e-005

Table 4a: 5YLU GC-MS CHARACTERIZATION

PUBCHEM CID	ENTRY NAME	DOCKING SCORE
439192	L- Sorbose	-6.408
15746013	Pentaborane	-5.335
322968	1-azabicyclo[2,2,2]octan-3one	-5.315
130564	Omeprazole	-5.200
528381	Misoprostol	-5.173
556801	Methyl-3,4-*O*-furylidene.beta.l-arabino	-5.116
8078	4,7-Methano-2H-inden-2-one	-5.041

Table 4b: 5YLU HPLC-MS QUANTIFIED COMPONENTS

PUBCHEM CID	ENTRY NAME	DOCKING SCORE
16218542	Rutin hydrate	-12.852
442428	Naringin	-9.019
5280343	Quercetin	-8.234
689043	Caffeic acid	-7.567
5280443	Apigenin	-7.300
370	Gallic acid	-7.230
5280863	Kaempferol	-7.153
445858	Ferulic acid	-6.671
637542	*p*-Coumaric acid	-5.936
338	Salicylic acid	-5.566

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130564	Omeprazole	-5.200
5282381	Misoprostol	-5.173

Table 4c: 6M9T GC-MS CHARACTERIZATION

PUBCHEM CID	ENTRY NAME	DOCKING SCORE
5282381	Misoprostol	-9.651
549023	4,7-Methano-2H-inden-2-one	-8.003
439192	L-Sorbose	-7.063
130564	Omeprazole	-6.421
91700912	Methyl-3,4-O-furylidene.beta.l-arabino	-5.900
15764013	Pentaborane	-5.230
322968	1-azabicyclo[2,2,2]octan-3one	-5.108
556801	2-Oxatricyclo[4,3,1,0(3,8)]decan-10-one	-5.087

Table 4d: 6M9T HPLC-MS QUANTIFIED COMPONENTS

PUBCHEM CID	ENTRY NAME	DOCKING SCORE
5280343	Quercetin	-8.746
5282381	Misoprostol	-8.553
5280863	kaempferol	-7.915
5280443	Apigenin	-7.584
130564	Omeprazole	-6.700
689043	Caffeic acid	-6.235
338	Salicylic acid	-6.184
445858	Ferulic acid	-6.048
370	Gallic acid	-5.739
637542	p-Coumaic acid	-5.414

GC-MS analysis showed that unripe *Musa sapientum* possessed different characters within the phytoconstituent with percentage abundance of each character. This proved that GC-MS can be used to detect compounds using the relative gas chromatographic retention times and elution patterns. The technique had been proved by studies to elute components of a mixture in combination with the mass spectral fragmentation patterns.[15]. This means that GC-MS technique might only be used to identify fragments contained in a phytochemical compound but not the compound itself, and the characteristic structure be identified through its peak. HPLC-MS analysis showed that *Musa sapientum* fruits possessed different phytoconstituents and the amount per contained in each compound. The phytoconstituents identified were mainly phenolic and polyphenolic compounds which had been proved in a study by [16]. Study by [18] had also prove *Musa sapientum* fruits to possess phytochemicals including flavonoids, rutin hydrates and naringins that played a crucial role in antioxidant defense mechanism and prevention of diseases [17,18]. This proved that HPLC-MS technique can identify and quantify phytoconstituents contained in a mixture. That was in agreement with the findings from[19] which suggested that the combination of HPLC technique and MS allowed the identification of compounds based on their unique mass-to-charge ratio, providing valuable information about their chemical structure and composition [19]. The amount per area of HPLC-MS identified components differed within fractions as well as their retention times. Comparing CE and all fractions with their standards (quercetin), p-Coumaric acid showed the highest retention time and the greatest amount per area across almost all fractions including CE. Statistical analysis showed that all phytoconstituents were statistically significant when compared with quercetin with p-value of 0.0001.

Molecular docking results obtained from GC-MS characterization fragments and HPLC-MS quantified phytoconstituents showed that quantified phytoconstituents had higher and better docking scores than characterization fragments and to an extent better scores than the two standard drugs. For 5YLU, a H/KATPase receptor, L-sorbose had highest affinity and more interaction than other fragments and the standard drugs including a proton pump inhibitor, Omeprazole, while rutin hydrate showed greater affinity, higher binding energy and interaction, followed by naringin and quercetin than both the standard drugs and other phytoconstituents. Studies had proved Musa sapientum's interaction with 5YLU receptor, [20]Showed that *Musa sapientum* fragments had more binding energy and better interaction with 5YLU receptor than Omeprazole [20]; In-silico studies carried out by[21] attested to the presence of Kaempferol, caffeic acid, gallic acid, quercetin, coumaric acid, naringin, hesperitin and salicylic acid in *Musa sapientum* pulp, the phytoconstituents having more interactions and more binding energies and their antioxidant/antiradical activities [21].

At 6M9T a PGE receptor, misoprostol showed higher affinity, greater binding energy and interaction compared with characterization fragments, but quercetin proved to be more effective with highest score proving higher affinity, greater binding energy and interaction with the receptor compared to misoprostol and other quantified phytoconstituents. Work by [5] had attested to misoprostol higher affinity than fragments at 6M9T receptor [5]. High docking scores obtained proved that *Musa sapientum* fruits contained phytochemicals responsible for its anti-ulcer activities hence the affinity and interactions with two different receptors implicated in ulceration. The mechanism might be attributed to the antioxidant and anti-inflammatory potentials leading free radical and reactive oxygen species eradication.

Conclusion

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This research had identified different fragments and phytochemicals responsible for anti-ulcer potentials of unripe *Musa sapientum* fruits through two powerful techniques, GC-MS and HPLC-MS. The docking results also proved that the identified compounds had affinity and interaction with receptors implicated in ulceration with HPLC-MS identified compounds having better interactions than GC-MS characterized fragments. The similarity in the docking scores of quercetin and misoprostol suggested a greater protective than healing potentials if these phytoconstituents should be integrated into drug discovery pipeline.

Conflict Of Interest

The authors declare no conflict of interest

Authors' Declaration

The authors hereby declare that the work presented in this article are original and that any liability for claims relating to the content of this article will be borne by us.

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