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Isolation of Bioactive Compounds in Allanblackia Floribunda Fruit and The Molecular Docking of The Compounds Against SARS-CoV-2 Variants

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Abstract: Compounds were isolated from the seed of *Allanblackia floribunda* using biologically guided chromatographic methods. Garcinia bioflavonoid (GB-1a and GB-2a), microdiplosone, and malic acid were isolated from the seed, pulp, and peel of the fruit. These compounds, even though they are known compounds previously isolated from another member of the Clusiaceae family, have not been isolated from *Allanblackia floribunda*. The structural elucidation of isolated compounds was done using IR, 1HNMR, 13C NMR, and MS spectroscopy. The molecular docking studies of compounds with SARS-CoV-2 variants (6M0J), omicron 2 (7T9L), and 6LU7 and subsequent comparison with molnupiravir and remdesivir known medications for SARS-CoV-2 showed that GB1a and GB2a had docking scores of -8.3 and -8.6 respectively which was close to that of molnupiravir (-8.3) but greater than that of remdesivir (-7.6). At the same time, that of microdiplodiasone and malic acid were lower than that of the two drugs. Also, GB1a and GB2a had better docking scores when docked with omicron 2 (7T9L) and 6LU7 than the reference ligands. These suggest that the compounds can be investigated further for the development of active drugs against SARS-CoV-2.

Keywords: *Allanblackia floribunda*, *Garcinia* bioflavonoids, SARS-CoV-2.

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1. INTRODUCTION

Allanblackia, a genus of flowering plants in the Clusiaceae family, is predominantly found in tropical regions. This family has 14 genera and trees of about 600 species that belong to this family have been identified (1). The *Clusiaceae* family is a known source of important secondary metabolites, which includes xanthones, coumarins, bioactive bioflavonoids, and some benzophenones, which are produced by the plants primarily for defense purposes are useful for several medicinal purposes in human (2-4).

Different parts of the plants have been investigated for their medicinal benefits, which were prompted by their local therapeutic uses. The bark is locally used against cough, dysentery, diarrhea, and toothache as an aphrodisiac and pain reliever. They are also known to have antihypertensive, anti-inflammatory, and hypoglycemic activities (5). The extracts are used to relieve smallpox, chicken pox, measles, scrotal elephantiasis, asthma, and bronchitis (1, 6). To alleviate painful joints, the body can also be rubbed with the pounded bark of Allanblackia floribunda (7,8). The fruit components have high antioxidant activities, which has encouraged its use as nutraceuticals (9). The seed has high fat and carbohydrate content, which plays an important role in body metabolism; it is also rich in essential minerals, especially calcium and magnesium (10,11).

Chemical constituents previously isolated from *Allanblackia* include Garcinol, cambogin, guttiferone F, and allanxanthone A, which were obtained from *Allanblackia monticola* fruits (12). Xanthenedione (Allanxanthone C), garciniafuran, tovophyllin A, rubraxanthone, norcowin, mangostin, and stigmasterol were also isolated from its stem bark (13). Xanthone derivative named allanxanthone E was isolated and characterized through phytochemical investigations performed on the seeds together with seven known compounds: 1,7-

dihydroxy-3-methoxy-2-(3-methylbut-2-enyl)xanthone, α-mangostin, garciniafuran, allanxanthone C, and 1,6-dihydroxy-2,4-diprenylxanthone, friedelin and lupeol (13,14).

Benzophones (hydrocotin, guttiferrone F) and xanthones (1,3,5-trihydroxyxanthone and 4,5-dihydro-1,6,7-trihydroxy-4′,4′,5-trimethoxyfurano-[2,3;3,4] xanthone) were identified in the heartwood of *A. floribunda* and *A.stuhlmanni* as well as bioflavonoids such as Moreflavone and Volkensiflavone (15). Allanxanthone A, 1,5-dihydoxyxanthone, 1,5,6-trihydroxy-3,7-dimethoxyxanthone, stigmasterol and stigmasteryl-3-O-b-d-glucopyranoside were isolated from the stem bark of *A. floribunda* (16). Funkugiside, morelloflavone, volkensiflavone I,7-dihydroxyxanthone, morelloflavone, and spicataside were also isolated from the stem bark and root (8).

Compounds useful as drugs to cure SARS-CoV-2, which posed a major challenge all over the whole in the year 2020, have been investigated by scientists, especially because of the discovery of different variants. Molnupiravir and remdesivir are potential drugs that can be used to inhibit SARS-CoV-2. In-vivo and in-silico approaches have been used to ascertain its effectiveness as potential drugs (17-19). Their use as drugs has reduced hospitalization of patients (19).

Trials conducted using 304 cases showed that molnupiravir has the potential to effectively decrease the mortality rate in patients diagnosed with COVID-19 within the moderate limit (20).

Also, research to find out drugs that are potent targets of specific diseases has recently been enhanced using molecular docking studies against possible target proteins (21). Rutin, ritonavir, emetine, and some other compounds have been investigated for their possible potency against SARS-CoV-2 protease (PDB: 6Y84 using molecular docking study (22-23). Some of these studies have provided positive outcomes that have brought about major advances in medicine and drug research.

The seed of *A.floribunda* is of great importance because of its seed oil, and no isolation has been reported from it. Therefore, in this work, the isolation and structural elucidation of four compounds were reported from the seed and their docking against different variants of SARS-CoV-2.

2. EXPERIMENTAL SECTION

2.1. Plant Material

A substantial amount of mature fruit from Allanblackia floribunda was harvested in a forest located at Igbara Odo Ekiti, situated in Ekiti State, Nigeria. Subsequently, this plant was authenticated and documented at the Department of Plant Science's herbarium unit at Ekiti State University with voucher number UHAE EPH 2:001.

2.2. Extraction and Isolation

The seeds, pulp, and the peel of the fruit were carefully separated, and the moisture content was removed by drying at room temperature for two weeks. The dried seed (3.60 kg) was milled using an electric blender (Marlex AC9829) and extracted with chloroform for three days in order to extract the oil content of the seed. The residue was further extracted using methanol for three days; the methanol extract was also decanted, filtered, and concentrated.

The methanol extracts of the seeds, due to their high antioxidant and microbial activity deduced from previous work, were fractionated using the column chromatography method. 80 g of the methanol extract of the seed was dissolved in methanol and adsorbed on silica gel (230-400 mesh), and the constituents were separated by column chromatography using 300 mL of the following solvents or solvent mixture in a step-wise gradient. In each case, the preceding solvent/solvent mixture was gradually enriched with the next solvents in the gradient. The solvent gradient was in the following order: *n-hexane* (100%), ethyl acetate in *n*-hexane (5, 10, 15, 20, 25…95%), ethyl acetate (100%), methanol in ethyl acetate (5, 10, 15, 20, 25…95%), and methanol (100%).

After being collected into test tubes, the fractions were evaluated using TLC analysis by spraying with vanillin-sulphuric acid. Those exhibiting similar Rf values were combined and resulted in a total of 32 dried fractions (labeled F1-F32). After passing through a mixture of EtOAc-n-hexane (90:10), F15 was subjected to column chromatography using silica gel and solvents, including n-hexane, ethyl acetate, and methanol, in the same manner. Similar fractions were combined, resulting in five (5) bulked fractions. TLC analysis revealed that some of these contained only one compound. Here, Compound I and compound II were obtained. F_{21} eluted with the mixture of EtOAc-methanol (75:25) was further separated using n-hexane, ethyl acetate, and methanol. The eluent was collected in test tubes, after which similar fractions were combined and evaporated, from which Compound 3 was isolated.

The chromatographic purification process used for the seed was repeated to purify 80 g of the crude methanol extract obtained from *A. floribunda* fruit pulp. 368 fractions were collected, which were later combined based on the TLC analysis into 17 fractions. Subsequent column chromatography was carried out until the desired pure compounds were obtained. A white crystal (compound IV) was discovered from fractions 8 and 9, which was properly filtered out and washed using ethyl acetate.

2.3. Spectroscopic Analysis

The spectroscopic details of the isolated compounds were investigated using Buker Platinum ATR mounted onto a Buker Tensor 27 FT-IR spectrometer, Agilent technologiesm1620 infinity series/Agilent quadrupole LCMS and the samples were run on Bruker 400MHz NMR spectrometer.

2.4. Plant Material *In silico* Analysis

2.4.1 Ligand preparation

The PubChem ID of the ligands (compounds 1- 4), molnupiravir, and remdesivir were obtained from PubChem. Chimera 1.14 was used to retrieve the structures based on their ID and subsequently save them in PDB format while minimizing optimal docking energy. Minimized compounds were uploaded to AutoDockTools-1.5.6 software, where the OpenBabel plugin was used for conversion into the PDBQT format.

2.4.2 Protein preparation

The crystal structures of required protein, SARS-CoV-2 main protease (Mpro: 6LU7), SARS-CoV-2 spike receptor-binding domain bound with ACE2 (6M0J) and Cryo-EM structure of SARS-CoV-2 Omicron spike protein in complex with human ACE2 (7T9L) were obtained from the RCSB protein data bank (www.rcsb.org) in PDB format.

To prepare the structures, the PDB format of the proteins was uploaded to Chimera 1.14 workspace; after eliminating non-standard residues like ions, water, and bounded ligands from the protein structure, it underwent structural minimization via Chimera 1.14's editing wizard. The process involved taking 100 steepest descent steps with a size of Ă=0.02 and then undergoing 10 conjugate gradient steps at a step size of Ă=0.02 as well with an additional interval update every ten times; this was carried out in total. The Gasteiger force field was used to assign charges and Polar hydrogen bonds was incorporated. Then, the protonation state of histidine was set with AutoDockTools-1.5.6 software. Upon completion, PDB files of the modified protein were saved in PDBQT format before being uploaded for molecular docking analysis using PyRx software.

2.4.3 Molecular Docking

To conduct the molecular docking of proteins and ligands, AutoDock Vina in the PyRx were used. The grid space was established by focusing on significant amino acid residues that were chosen from UniProtKB. Grid box size, center (29.7237, 11.7994, 42.1527)Å and size (38.2112, 26.7617, 36.1823) Å, x, y and z respectively were set for Mpro 6LU7. Also, Grid box size, center (x -51.8334 Å, y -35.9153 Å and z 4.4678 Å) and size (x 69.4516, y 62.4510 and z 69.1699) were set for SARS-CoV-2 spike RBD (6MOJ) and SARS-CoV-2 spike RDB omicron variant (7TqL) Grid box size was set at center (x 226.1996 Å, y 176.1916 Å and z 236.6954 Å) and size (x 35.0793, y 42.4635 and z 67.3292).

3. RESULTS AND DISCUSSION

3.1. Structural Elucidation

3.1.1. Compound I

Compound I (GB-1a) is an amorphous yellow solid with a melting point of 200 ºC. The IR showed absorption bands at 3187 cm^{-1} and 1733 cm^{-1} for a carbonyl group. The mass as revealed by the LC-MS is m/z 542 with molecular formula $C_{30}H_{22}O_{11,}$ the fragmentation at m/z 541 [M^+ - H], 415, 288, 261, 141, 113, 112. The H NMR spectrum showed C-5 (OH) signal at δ 2.01 (s, 1H) and other OH at 0.89 (d, J = 7.0 Hz, 1H) , also, there was a presence of doublets at δ 7.38 (d, J = 2.2 Hz, 1H), 7.09 (d, J = 8.6 Hz, 1H), 5.62 (d, J = 11.9 Hz, 1H), 5.49 (d, J = 9.8 Hz, 1H), 5.15 (d, J = 13.0 Hz, 1H), 4.59 (d, J = 11.1 Hz, 1H). This result is in close agreement with those reported by Jackson et al. (1971) (24) for GB-1a (Table 1). The ^{13}C NMR (100 MHz, MeOD) showed signal at δ 197.52, 196.44, 166.56, 164.13, 163.42, 161.16, 157.24, 145.00, 130.42, 128.52, 121.69, 117.93, 115.61, 115.05, 114.39, 113.23, 112.79, 101.83, 101.24, 95.95, 94.88, 81.78, 79.16, 42.67 which is in agreement with those reported by Agrawal (1989) (25) (Table 2). Although this compound has been previously isolated from *Garcinia bsrchananir* and *Clusia columnaris* Engl, the isolation of GB-1a [(2S,2'R,3R)-5,5',7,7'-tetrahydroxy-2,2'-bis(4-hydroxyphenyl)-[3,8'-bichroman]-4,4'-dione] (1) from *A. floribunda* seed for the first time has been reported here.

3.1.2. Compound II

Compound II is an amorphous yellow solid with a melting point of 200 °C. The IR showed absorption bands of OH at 3185 and 1633 cm^{-1} for a carbonyl group. The Mass, as revealed by the LC-MS, is m/z 298 with molecular formula $C_{14}H_{14}O_{6,}$ the fragmentation at m/z, 261, 142, and 141. The ^1H NMR (400 MHz, MeOD) showed signal at δ 7.31 (s, 1H), 7.26 (d, J = 8.4 Hz, 1H), 7.11 (d, J = 8.3 Hz, 2H), 6.87 (d, J = 8.4 Hz, 1H), 6.65 (d, J = 7.4 Hz, 1H), 6.58 (d, J = 7.7 Hz, 1H), 6.52 (s, 1H), 6.43 (d, J = 8.3 Hz, 1H), 6.36 (s, 1H), 6.27 (s, 1H), 6.08 (s, 1H), 5.99 (d, J = 11.7 Hz, 1H), 5.74 (d, J = 11.9 Hz, 1H), 5.65 (d, J = 12.0 Hz, 1H), 4.09 (q, J = 7.1 Hz, 1H), 2.01 (s, 1H), 1.25 – 1.17 (m, 1H (Table 3). The ^{13}C NMR (100 MHz, MeOD) showed signal at δ 13C NMR (101 MHz, MeOD) δ 196.77, 182.44, 166.78, 164.31, 163.45, 149.47, 145.28, 127.89, 119.32, 114.25, 102.02, 98.56, 81.41, 13.09 (Table 4). The compound isolated was elucidated as microdiplodiasone[(R)-2-ethyl-5,7-dihydroxy-2-((R)-5-oxotetrahydrofuran-2-yl)chroman-4-one] (2) when compared with those reported by Siddiqui et al. (2011) (26).

3.1.3. Compound III

Compound III (GB-2a) is an amorphous yellow solid with a melting point of 210 ºC. The IR showed an OH absorption band at 3222 and 1643cm^{-1} for a carbonyl group. The Mass as revealed by the LC-MS is m/z 558 with molecular formula $C_{30}H_{22}O_{11,}$ the fragmentation at m/z 599 [M^+ + 1], 421, 295, 268, 153, 141, 113, 112. The ^1H NMR spectrum showed C-5 (OH) signal at 2.16 (s, 1H) and other OH at 1.27 (s, 1H); also, there was a presence of doublets at 3.41 (d, J = 9.0 Hz, 5H), 5.16 (d, J = 7.6 Hz, 1H), 5.34 (d, J = 13.6 Hz, 1H), 6.86 (d, J = 6.5 Hz, 1H), 7.30 (s, 2H). This result is in close agreement with those reported by Jackson et al (1971) (24) (Table 1). The ^{13}C NMR (101 MHz, MeOD) showed a signal at δ 81.5, 49.6, 196.5, 163.4, 95.9, 164.3, 94.6, 161.2, 102.7, 105.1, 129.4, 128.5, 156.9, 114.1 and 128.5 which is in agreement with those reported by Agrawal (1989) (25) (Table 2) for GB-2a [2'-(3,4-dihydroxyphenyl)-5,7,7'-trihydroxy-2-(4-hydroxyphenyl)-[3,8'-bichroman]-4,4'-dione] (3). Although this compound has been previously isolated

from *Garcinia bsrchananir* and *Clusia columnaris* Engl, the isolation of GB-2a (Figure 1) from *A.floribunda* seed for the first time is been reported here, but (27) had earlier confirmed the presence of GB-2a in an investigation carried out on the seed extract of *A. floribunda* using HPLC-PDA-ESI/MS.

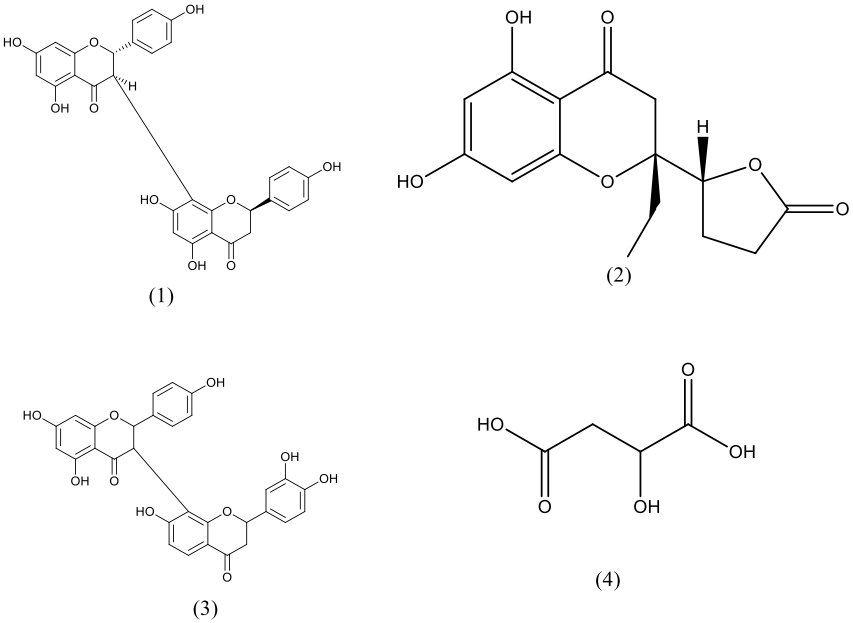

Figure 1: Isolated Compounds from *A. floribunda*.

3.1.4. Compound IV

Compound IV is a white powder with a melting point of 130 °C. The IR showed OH absorption bands at 3397 and 1713 cm^{-1} for a carbonyl group. The molecular weight is 134 with the molecular formula $C_4H_6O_5$. The NMR showed ^1H NMR (600 MHz, MeOD) δ 4.83 (s, 1H), 2.93 (d, J = 15.4 Hz, 1H), 2.81 (d, J = 15.4 Hz, 2H) and ^{13}C NMR (150 MHz, MeOD) δ 175.04 (-COOH), 170.67 (-COOH), 50.76 (-CH), 42.62 ($-CH_2$) which is in agreement with results reported by Kosir et al. (1998) (28) for malic acid (4) (Table 5).

Table 1: ^1H Nuclear Magnetic Resonance results obtained for of Compound I and III.

^1H				
Assignment	**Compound I**	**GB-1a** Jackson et al (1971) (24)	**Compound III**	**GB-2a** Jackson et al (1971) (24)
C-5 OH	2.01 (s, 1H)	2.05 (s, 1H)	2.16 (s, 1H)	2.31 (s, 1H)
2.44 (s, 1H)				
Other OH	0.89 (t, J = 7.0 Hz, 1H)	0.90 (s, 1H)	1.27 (s, 1H)	1.44 (s, 4H)
C_6 ring	4.59 (d, J = 11.1 Hz, 1H)	4.27	3.95 (d, J = 11.6 Hz, 3H)	4.10 (s, 3H)
C_2/C_6	2.53 (d, J = 17.5 Hz, 1H)	2.98 (d, 2H J=9.0)		
3.05 (d, 2H J=9.0)	3.53 (d, J = 8.7 Hz, 2H),			
	2.82 (d, J = 11.1 Hz, 2H)			
C_3/C_5	4.59 (d, J = 11.1 Hz, 1H)			
	3.39 (d 2H J=9.0)			
3.48 (d 2H J=9.0)	3.41 (d, J = 9.0 Hz, 5H)	3.08-3.20 (d, 5H)		
C_2/C_3 (Ring 1-C)	5.62 (d, J = 11.9 Hz, 1H	4.54 (d 1H J=12.0)	5.16 (d, J = 7.6 Hz, 1H)	4.71 (d, J = 12 Hz, 1H)
(Ring I-C)	5.62 (d, J = 11.9 Hz, 1H)	5.55 (d 1H J=12.0)	5.34 (d, J = 13.6 Hz, 1H)	5.32 (d, J = 12 Hz, 1H)
C_2(Ring II-C)	5.49 (d, J = 11.8 Hz, 1H)	4.75 (d 1H J=12.0)	6.86 (d, J = 6.5 Hz, 1H)	4.30 (d, J = 12 Hz, 1H)
C_3(Ring II-C)	7.38 (d, J = 11.6 Hz, 1H)			
7.09 (d, J = 11.6 Hz, 1H)	7.10 (d 1H J=12.0)			
7.59 (d 1H J=12.0)	7.30 (s, 2H)	6.91 (d, J = 12 Hz, 1H)		
7.35 (d, J = 12 Hz, 1H)				

Table 2: The data obtained from the ^{13}C NMR analysis of Compound I and III.

^{13}C NMR	Compound I	GB-1a Agrawal (1989) (25)	Compound III	GB-2a Agrawal (1989) (25)
C-2	81.8	81.4	81.5	81.7
C-3	42.7	47.7	49.6	51.0
C-4	196.4	195.2	196.5	197.2
C-5	164.1	163.4	163.4	164.6
C-6	95.9	96.0	95.9	93.3
C-7	166.6	165.9	164.3	164.9
C-8	94.9	95.0	94.6	93.1
C-9	163.4	162.3	161.2	162.1
C-10	101.2	101.0	102.7	162.1
C-1′	128.5	127.9	105.1	105.8
C-2′	130.4	128.5	129.4	130.3
C-3′	114.4	114.5	128.5	128.2
C-4′	157.2	157.1	156.9	159.2
C-5′	113.2	114.5	114.1	113.2
C-6′	128.5	128.5	128.5	128.2

Table 3: ^{1}H NMR spectral assignments of Compound II.

1H Assignment	Compound II	Siddiqui et al. (2011) (26)
5-OH	7.31 (s, 1H)	11.57 (s, 1H)
7-OH	7.26 (d, J=8.4 Hz, 1H)	11.45 (s, 1H)
H-8	7.11 (d, J=8.4 Hz, 1H)	7.21 (brs, 1H)
H-6	6.87 (d, J=8.4 Hz, 1H)	7.11 (brs, 1H)
H-9	5.99 (d, J=11.7 Hz, 1H)	4.58 (t, 1H)
H-3α	5.74 (d, J=11.9 Hz, 1H)	2.98 (d, J=17.1Hz, 1H)
H-3β	5.65 (d, J=12.0 Hz, 1H)	2.61 (d, J=17.1Hz, 1H)
H-11	4.09 (m, 2H)	2.60 (m, 2H)
H-10	2.01 (m, 2H)	2.32 (m, 2H)
H-13	1.25 (s, 3H)	1.43 (s, 3H)

Table 4: ^{13}C Nuclear Magnetic Resonance analysis result for compound II.

^{13}C NMR	Compound II	Siddiqui et al. (2011) (26)
C-4	196.77	196.6
C-12	182.44	176.6
C-5	166.78	166.0
C-7	164.31	161.2
C-8a	163.45	158.2
C-4a	149.47	109.3
C-6	145.28	110.6
C-8	127.39	108.9
C-9	81.77	82.7
C-2	81.41	81.1
C-3	42.67	42.8
C-11	29.38	28.1
C-10	22.44	22.2
C-13	18.09	18.8

Table 5: The compound IV ^{13}C NMR result.

^{13}C NMR	Compound IV	Kosit et al. (1998) (28)
-COOH	175.04	178.0
-COOH	170.67	178.0
-CH	50.76	69.9
-CH	42.62	41.3

3.2. Molecular Docking

The molecular docking studies of ligands (Table 6) with the omicron Variant (6M0J) and subsequent comparison with molnupiravir and remdesivir, a known medication for SARS-CoV-2 (Figure 2), showed that GB1a and GB2a had docking scores of -8.6 and -8.3 Kcal mol^{-1} respectively which was close to that of molnupiravir (-8.3 Kcal mol^{-1}) but greater than that of remdesivir (-7.6 Kcal mol^{-1}), while that of microdiplodiasone and malic acid were lower than that of the two drugs. Also, GB1a and GB2a revealed better docking scores when docked with omicron 2 (7T9L) and 6LU7 than the reference ligands. Microdiplodiasone had docking scores similar to the reference ligands in the target proteins (-6.1 and -6.8 Kcal mol-1), and malic acid had a lower value

compared to other ligands. The binding of the ligands with the omicron Variant (6M0J) had the best binding energy as the ligand formed a firm bond with it. The binding with GB1a formed hydrogen bond interaction with ALA 43, GLU 42, TYR 53, ASN 147, GLU 24, MET 138, ASP 101, ARG 108, PRO 107, pi-pi interaction with ALA 136, ALA 146, ALA 105. Van der Waal's interaction with ARG 113, ASN 103 (Table 7) which was closely related to the binding of 6M0J with molnupiravir and remdesivir. GB2a had hydrogen bond interaction with ARG 113 and TYR 53, pi-pi interaction with ALA 146 and Van der Waal's interaction with GLU 24 and ARG 108. Malic acid only formed hydrogen bond interaction with THR 72, ARG 99 and HIS 110 when it was docked with omicron variant (6M0J).

Therefore, GB1a and GB2a with better docking scores than the reference ligands and similar target sites can be useful ligands in the design of anti-COVID drugs and vaccines.

Table 6: The molecular docking result of isolated compounds with different variant of COVID-19.

	Ligand	Binding Energy (Kcal mol^{-1})		
		6LU7	6M0J	7T9L
A	GB-1a	-6.6	-8.6	-7.3
B	GB-2a	-6.7	-8.3	-7.4
C	Malic acid	-4.3	-4.9	-4.7
D	Microdiplodiasone	-6.1	-6.8	-6.8
E	Molnupiravir	-6.1	-8.3	-6.5
F	Remdesivir	-6.2	-6.8	-7.6

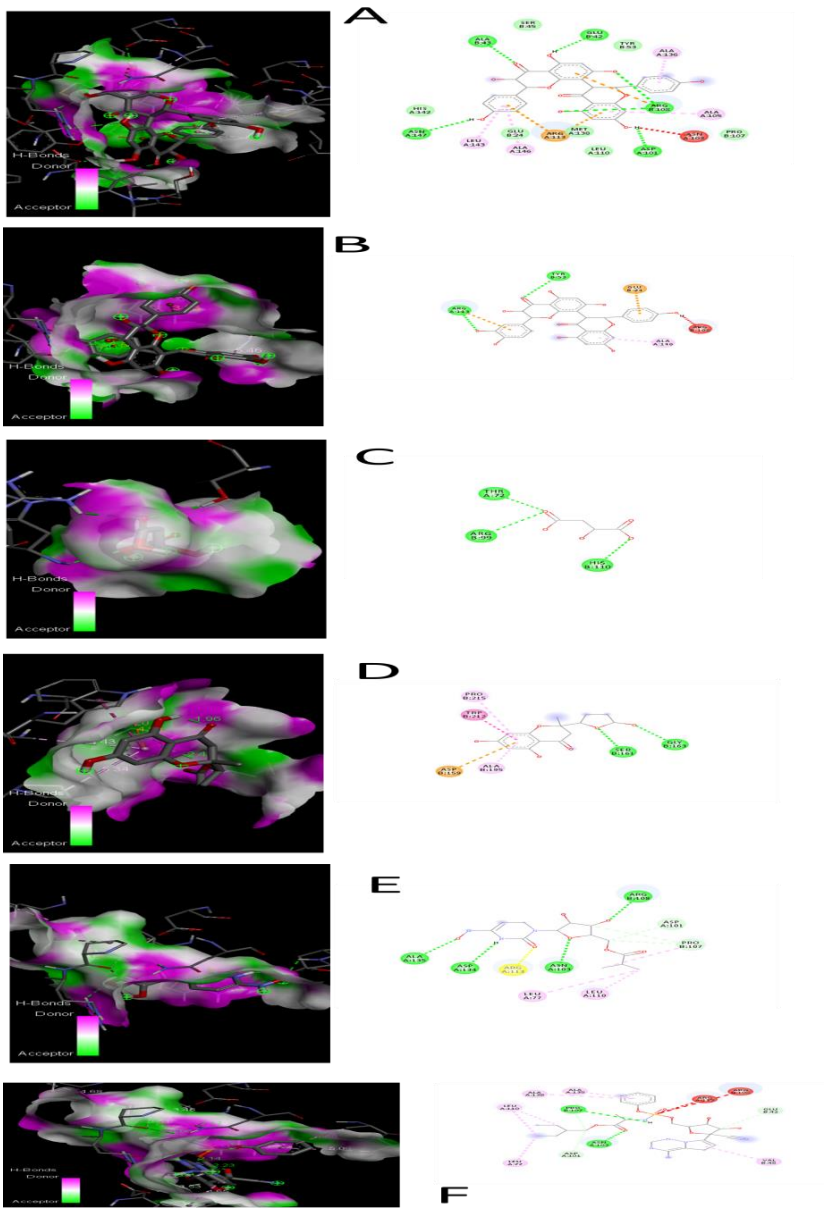

Figure 2: Molecular docking result of Isolated compounds (A-C), molnupiravir (D), and remdesivir (F) against SARS-CoV-2 spike receptor-binding domain bound with ACE2 (6M0J).

Table 7: Molecular docking result of Isolated compounds (A-C), molnupiravir (D), and remdesivir (F) against SARS-CoV-2 spike receptor-binding domain bound with ACE2 (6M0J).

Compounds	Binding Affinity	H-Bonds	Amino acid interaction	
			Hydrophobic/Pi-cation/Pi-anion/ Pi-alkyl interactions	Van der Waals interactions
GB-1	-8.6	ALA 43, GLU 42, TYR 53, ASN 147, GLU 24, MET 138, ASP 101, ARG 108 PRO 107	ALA 136, ALA 146, ALA 105.	ARG 113, ASN 103.
GB-2	-8.3	ARG 113, TYR 53	ALA 146	GLU 24, ARG 108
Malic acid	-4.9	THR 72, ARG 99 HIS 110		
Microdiplodiasone	-6.8			
Molnupiravir	-8.3	ALA 135, ASP 134, ARG 113, ASN 103, ARG 108	LEU 77, LEU 110	ASP 101, PRO 107
Remdesivir	-6.8	PRO 107, ASN 103, ASP 101, GLU 42	LEU 110, ALA136, ALA 135, LEU 77, VAL 48	ARG 113, AER 108

4. CONCLUSION

The extraction and isolation of the chemical component of *Allanblackia floribunda* fruit led to the isolation of four known compounds: GB-1a, GB-2a, Malic acid, and Microdiplodiasone. The molecular docking of these compounds with SARS-CoV-2 (6LU7), Omicron 1 (6M0J), and Omicron 2 (7T9L) showed good docking scores when compared to molnupiravir and remdesivir as reference drugs. Hence, these compounds can be investigated further for their drug ability and toxicity against human cells.

5. CONFLICT OF INTEREST

There are no conflicts to declare.

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