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Interactions of HRLCMS-QTOF Detected Plant Metabolites of *Abrus precatorius* L. Seeds with EGFR and the Effect of Classically Detoxification Process

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Abstract

Abrus precatorius L. is one of the most important medicinal plants with toxic principles which has been reported for many cases of poisoning throughout the globe. *Shodhana* is an important technique in Ayurveda which includes a set of procedures to detoxify the toxic herbal raw drugs. Hence three varieties of unprocessed and *shodhana* processed *Abrus precatorius L.* seeds were chosen and the hydro alcoholic extracts were prepared by maceration. These extracts were subjected to HRLCMS-QTOF analysis and the receptor-specific action of all the major components selected with the cutoff range of more than $0.2x10^6$ counts was analyzed with GLIDE (Schrodinger 2021-1, maestro v13.6) software. Totally 570 molecules were identified in HRLCMS, and 299 molecules were docked against EGFR downloaded from the RCSB database with the crystal structure of 5XDK. The HRLCMS has revealed the presence of many unknown compounds in extracts and the major compounds identified were Indoleacrylic acid, PABA, Galangin 3- [galactosyl-(1->4), Chrysoeriol 7-O-neohesperidoside, gallic acid, calendoflaside, etc. In docking studies, the glide scores of the ligands were compared with the standard ligand 8JK and it was found that the compounds present in the extracts have shown good binding scores in comparison with the standard ligand. It is concluded that the *shodhana* processed seed extracts show a wide range of phytochemical variation and a notable *in silico* docking score and hence the raw drug after *shodhana* can be considered promising for research and development of cancer management therapies.

Keywords: *Abrus precatorius*, Docking, HRLCMS, Plant Metabolite Evaluation, *Shodhana*

1. Introduction

Abrus precatorius is a flowering herbaceous climber native to South Asia, belongs to the Fabaceae family and is commonly called crab's eye, love pea, rosery pea, jequirity, prayer bead, gunja etc. The occurrence of this plant is commonly seen in tropical regions and hence its distribution is widely pan-tropical. This plant is considered one of the most highly invasive due to the potent plant poison named abrine. This plant poison is a dimer which is made up of two protein subunits A and B[1]. This protein was reported to prevent protein synthesis by acting upon 28S RNA and each molecule may inactive up to 1500 ribosomes per second. Abrin is considered highly toxic having an LD_{50} of

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0.56 µg/kg in mice and an average lethal dose of 0.1mg in humans[2]. The poisoning symptoms following consumption of the broken seeds of *Abrus precatorius* include nausea, vomiting, liver failure, convulsions, and death after several days[2]. Even though this plant was found to be highly toxic, no report was found regarding the occupational poisoning. The seeds of this plant are used for various other purposes such as measuring gold and the weight of 1 seed is called *Ratti* in the Ayurvedic system of medicine. The approximate weight of 8 *Ratti* is 1 gram. These seeds are found to be highly useful in the preparation of various medicines in different parts of the world[3-7]. In the Indian classical system, the seeds are subjected to a detoxification process before being used in medicinal preparations and the detoxification process is called *Shodhana*. The drugs which are subjected to the detoxification process are supposed to possess a wide range of activities and hence used in various pathological conditions[8]. Cancer is one such pathological health condition which needs more active drugs, and researchers are nowadays focusing on active herbal remedies. Target target-based approach is considered one of the most effective ways of finding cures for cancer. Among the various targets, the epidermal growth factor receptor is the most important one to focus on. EGFR is a receptor for members of the epidermal growth factor family. It binds to epidermal growth factor and leads to dimerization of receptor and tyrosine autophosphorylation that leads to cell proliferation. The mutations that occur in these genes may lead to various cancers such as pancreatic cancer, lung cancer, liver cancer, colorectal carcinoma, breast cancer, ovarian cancer, bladder cancer, skin cancer and thyroid cancer[9]. EGFR play a vital role in the pathogenesis of various cancers and 90% of pancreatic cancer cases reveal a high expression of EGFR that is associated with poor prognosis. When these receptors are amplified it leads to more expression on the cell surface which results in uncontrollable cell growth and division. In most cases, the transformation of normal cells to cancer cells may occur and it may provide suitable conditions for cancer cell survival. Various drug researchers are currently in progress in various parts of the world for controlling EGFR expression and EGFR-based cancer management[10].

2. Materials and Methods

2.1 Collection of Raw Drugs

Red, white, and black varieties of *Abrus precatorius* L. seeds were collected from Siddha Medicinal Plants Garden, Central Council for Research in Siddha, Government of India, Mettur, Salem. The collected seeds were identified by Dr P. Radha, Research Officer (Botany), SMPG, Mettur and further the herbarium was assigned with the reference voucher specimen numbers 1920, 1924 and 1935 for the red, black, and white varieties respectively.

2.2 Shodhana and Preparation of Extracts

The seeds were subjected to the classical detoxification technique of *shodhana* using the fermented supernatant of polyherbal rice gruel called Kanjika which was prepared by mixing various herbal ingredients such as turmeric powder, dry ginger powder, mustard seed, cumin seeds, asafoetida pieces fried in ghee, red rice (half boiled), horse gram, black gram, mustard seed oil, rock salt, bamboo leaves and radish along with distilled water[11]. All the ingredients were sealed in an air-tight glass container for 15 days and the fermented supernatant was collected. Then the seeds were processed by submerging and boiling in Kanjika for 3 hours. After boiling, the seed coats were removed and the seeds were shade-dried to complete the process[12,13]. Following that, the raw seeds along with seed coats and shodhana processed seeds shown in Figure 1 were coarsely powdered and subjected to extended maceration in 75:25 Ethanol: Water with frequent shaking for 48 days to facilitate the maximum extraction of phytoconstituents[14-17]. Post-maceration, the solvents were filtered and dried at room temperature.

2.3 HRLCMS-Based Plant Metabolite Profiling

2.3.1 Instrument Conditions

Seed extracts of all six seeds (three raws and three processed) were subjected to High-Resolution Liquid Chromatography Mass spectrophotometry and Quadrupole Time of Flight (HRLCMS-QToF) analysis for qualitative estimation of plant metabolites at Sophisticated Analytical Instrument Facility, IIT, Mumbai. The analysis was done using a 1290 Infinity UHPLC System, 1260 Infinity Nano HPLC with Chipcube, and 6550 iFunnel Q-TOFs, Agilent Technologies, USA. The analysis was performed in both positive and negative ion modes using Dual AJS ESI Ion Source. MS Absorbance threshold was fixed at 200 and MS/MS absorbance threshold was fixed at 5 and then the percentage relative threshold was fixed at 0.010 and the QTOF stop time was fixed at 25 minutes. For MS2 the scan rate was set at 1.00 spectra/sec and the m/z range was fixed at 120-1200. For precursor selection,

the percentage purity cutoff and absorbance threshold were set at 30% and 10000 respectively. Under source parameters, the gas temperature was kept at 250°C with a flow rate of 13 litre/min at 35 psig nebuliser pressure. The samples were drawn and ejected using the HiP sampler (Model: G4226A) at a speed of 100.0 µL/min. The scan source parameter values are Vcap 3500, Nozzle Voltage 1000 V, Fragment 175, Skimmer 65, and Octopole RF Peak 750.

2.3.2 Solvent System Composition and Column Condition

The elusion was performed with 0.1% formic acid in water (solvent A) and 90% acetonitrile+10% water + 0.1% Formic acid (solvent B). The elusion was performed in a gradient mode of 95:5% A: B at 0-1 min, 100% B at 1-25 min and 95:5% A: B at 25-30 mins with a flow rate of 0.300mL/min with Binary Pump (Model: G4220B) at 1200.00 bar pressure.

The C18 Column (Hypersil gold C18 100 x 2.1 mm^{-3} micron) was used in the G1316C column compartment at a temperature of 40°C and the analysis was performed at the wavelength of 254 to 360 nm. The molecules were analysed with the SAIF- IIT Bombay database and the name structure molecular weight, and mass-to-charge ratio of the molecules were determined[18].

2.4. Molecular Docking

For docking studies, the PDB 3D structure of epidermal growth factor receptor was downloaded from the RCSB website with the PDB id: 5XDK and resolution of 2.35 Å. It is a crystal structure of EGFR from the amino acid sequence of 696 to 1022, T790M in complex with CO-1686. This structure has two chains, which are chain A of 331 amino acid length and chain B of ligand. 8JC is commonly called Rociletinib (Drug bank id: DBW1907) which has been used for the prevention of non-small cell lung cancer in trials. The docking studies were conducted using GLIDE (Schrodinger 2021-1, maestro v13.6) software for the preparation of protein structure, targeting the binding site, grid formation and acquisition of docking score. The active site grid was formed with the major amino acids in a sequence that interacts with the receptor. The compounds identified using the HRLCMS analysis with the peak height of $0.2x10^6$ counts in individual extracts were selected and docked with the target protein to find the drug interaction score (Glide score) to analyse the binding efficiency of individual molecules in comparison with the standard ligand[19-21].

3. Results

3.1 HRLCMS Evaluation

The HRLCMS studies reveal a good variation in the metabolite profiles of the processed and unprocessed seeds. It explains the efficiency of the *shodhana* process in altering the phytochemical levels in raw drugs. The HRLCMS outcomes of red seeds, processed red seeds, white seeds, processed white seeds, black seeds and processed black seeds are shown in Tables 1 to 6. As a part of the outcomes, the details such as RT, start and end of the peaks and height of peaks were obtained. Based on these chromatogram details, the peak areas were calculated using the formula ½*(end-start of peak) *height and the percentage areas were calculated to analyse the major phytoconstituents in the extracts. The percentage areas of molecule peaks detected in each unprocessed and processed seed extract were compared in Figures 2 to 4. These results explain the qualitative and partially quantitative details of various phytochemicals in various extracts.

3.1.1 Unprocessed and Processed Red Seeds

In the hydro-alcoholic extract of unprocessed red seeds of *Abrus precatorius* total of 102 metabolites with valuable areas were obtained. Among them 21 compounds were unknown. In the positive ion mode, 60 compounds were observed, and the major compounds were indol acrylic with the percentage area of 11.58, Chrysoeriol 7-O-neohesperidoside 9.49%, PABA 7.84%, Galangin 3- [galactosyl-(1->4)- 6.18%, 6-Methylquinoline 4.15%, LysoPE (24:0/0:0) 3.95% and Isobutyl N-methylanthranilate 3.66%. In the negative ion mode, the major compound was found to be Gallic acid with a percentage area of 16.68. The other major compounds were the unknown compounds 1.20 and 1.21 with a percentage area of 9.65 and 5.67 respectively. Tenitramine 3.36% and 2-galloylglucose 3.14% were found to be the next major compounds.

In the extract of processed red seeds, a total of 100 compounds were found. 56 compounds were detected in positive ion mode and 44 compounds were detected in negative ion mode. In the positive ion mode, the major compound is unknown 2.7 with a percentage area of 19.46.



Figure 1. Three varieties (red, black, and white) of *Abrus precatorius* L. seeds in unprocessed and processed forms.

Next to that, the major compounds were Calendoflaside, unknown compound 2.6, 23-Acetoxysoladulcidine, and Mycinamicin VII with the percentage areas of 5.65, 5.07 and 4.34 respectively. In negative ion mode, the major compound was the unknown compound 2.18 with an 11.29% area at RT 18.615. Next to that gallic acid, 6-beta-D-Glucopyranosyl-4',5- dihydroxy-3',7-, hydroquinone, piperidine and unknown compound 2.15 were the major compounds with percentage areas of 9.71, 5.36, 4.09, 3.40 and 3.09 respectively.

The percentage areas of various molecule peaks detected in unprocessed and processed red seeds by HRLCMS were compared in Figure 2. The details of the compounds detected in the unprocessed and processed red seed extracts including abundance and scores were given in Tables 1 and 2.

3.1.2 Unprocessed and Processed White Seeds

In the unprocessed white seed extract, 97 metabolites were detected. Among them, 43 were detected in positive ion mode and 54 in negative ion mode. This is the only extract in which the number of molecules detected in negative ion mode is more in number than the molecules detected in positive ion mode. In the white seed extract the major compound found was indole acrylic acid with a percentage area of 13.62. Next to that, the major compounds were N-acetyl serotonin (11.92%), Unknown compound 3.8 (11.11%), Erinacine P (9.09%), Calendoflaside (5.92%) and Oleoyl Ethanolamide (4.69%). In the negative ion mode, the major compound found was Chrysoeriol 7-O-neohesperidoside (18.16%) and then Pipercitine (6.60%), Tenitramine (6.17%) and Pipericine (4.59%).

In the processed white seed extract total of 78 compounds were detected including 39 molecules in both positive and negative ion modes. In the positive ion mode, the major compounds found were N-Acetylserotonin (16.70%), Azobenzene (12.73%), Indoleacrylic acid (12.63%), Mycinamicin VII (12.24%), Erinacine P (7.37%) and Evodiamine (4.07%). In the negative ion mode, the major compounds were LysoPE (18:1(11Z)/0:0) (39.91%), Sambutoxin (12.985%), Chrysoeriol 7-O-neohesperidoside (9.48%), Tenitramine (7.67%) and Gallic acid – (3.01%).

The percentage areas of various molecule peaks detected in unprocessed and processed white seeds by HRLCMS were compared in Figure 3. The details of the compounds detected in the unprocessed and processed white seed extracts including abundance and scores were given in Tables 3 and 4.

3.1.3 Unprocessed and Processed Black Seeds

In the unprocessed black seed extract a total of 98 metabolites were detected. Among these 60 molecules were detected in positive ion mode and 38 molecules were detected in negative ion mode. In the positive ion mode, the major compounds were Calendoflaside (11.99%), Erinacine P (7.35%), Anthranilic acid (7.316%), Indoleacrylic acid (5.47%), N-Acetylserotonin (4.65%), Oleoyl Ethanolamide (4.39%), Unknown Compound 5.11 (4.255%) and Unknown Compound 5.9 (4.03%).

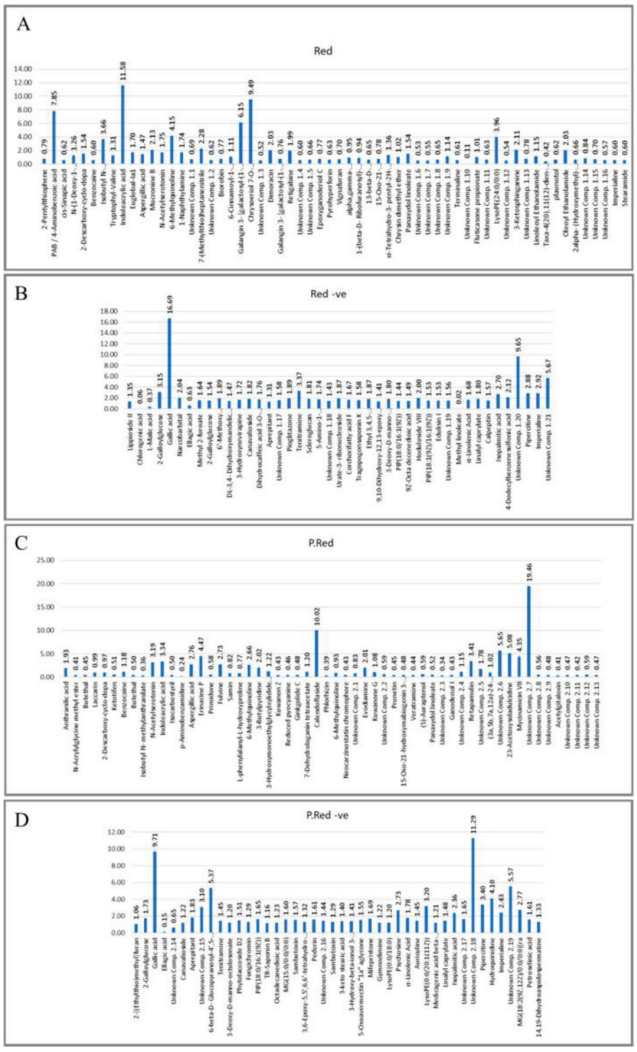


Figure 2. Percentage areas of various metabolites present in hydroalcoholic extracts of unprocessed and processed *Abrus precatorius* L. Red seeds. **(A)** Red seed extract (positive ion mode), **(B)** Red seed extract (negative ion mode), **(C)** Processed red seed extract (positive ion mode) and D-Processed red seed extract (negative ion mode).

In the negative mode, the major compounds were Gallic acid (16.99%), Unknown Compound 5.19 (13.26%), Petroselinic acid (6.48%), Tenitramine (5.208%) and 2-Galloylglucose (3.36%).

In the processed black seed extracts 94 compounds were detected. Among them, 52 compounds were detected in positive ion mode and 42 in negative ion mode. In the positive ion mode, the major compounds detected were unknown compound 6.6 (15.077%), Chrysoeriol 7-O-neohesperidoside (9.17%), Mucronine B (4.78%), Azobenzene (3.96%), Retigabine (3.88%), Indoleacrylic acid (3.78%) and 7-(Methylthio) heptane nitrile (3.69%). In the negative ion mode, the major compounds detected were Hydroquinidine (9.57%), 6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone (9.50%), Gallic acid (9.25%), Unknown Compound 6.12 (6.74%) and 14,19-Dihydroaspidospermatine (3.719%).

The percentage areas of various molecule peaks detected in unprocessed and processed black seeds by HRLCMS were compared in Figure 4. The details of the compounds detected in the unprocessed and processed black seed extracts including abundance and scores were given in Tables 5 and 6.

3.2 Molecular Docking

Through molecular docking analysis, the ability of all the secondary plant metabolites to fit into the active site of the EGFR (5XDK) shown in Figure 5 was analysed and the docking scores are represented in the form of glide score values represented in Table 7. The secondary plant metabolites with the top five glide g score values in each extract were observed along with their interactions at the target site and sorted in the descending order of receptor interaction (lesser glide score represents more binding with the target site) in Table 8. The presence of the top active metabolite of one extract in another was also mentioned.

In the red seed extract the top five metabolites with more prominent gscores are ellagic acid, 6'-Methoxy polygoacetophenoside, Chrysoeriol 7-O-neohesperidoside, PIP (18:0/16:1(9Z)) and Biorobin. Whereas in processed red seed extract the top five metabolites are ellagic acid, PIP (18:0/16:1(9Z)), phlorhizin, thyroxine sulfate and isocarbostyril. This kind of variation in the higher active molecules between the processed and unprocessed extracts was seen in other extracts also. In white seen extract Chrysoeriol 7-O-neohesperidoside, 6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone, Phloroacetophenone 6'-[xylosyl-(1->6)-glucoside], Paeonolide and 2-[3-Ethyl-5-(4-methoxyphenyl)-1H-pyrazol-4-yl] phenol was observed. But in processed white seed extract the top five molecules detected were Chrysoeriol 7-O-neohesperidoside, cis-Miyabenol C, Nicotiflorin, Biliverdin-IX-α and Isorhamnetin 3-O-[b- D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]. In black seed extract top five molecules such as Pallidol 3-glucoside, PIP (18:0/16:1(9Z)), calendoflaside, indoleacrylic acid and prunetin were turned into ellagic acid, Chrysoeriol 7-O-neohesperidoside, 6-beta-D-

Table 1. HRLCMS QTOF Compounds list of hydroalcoholic extract of *Abrus precatorius* L. red seeds

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
1	2-Pentylthiophene	$C_9H_{14}S$	177.0694	0.35	10345	75.5	Lippioside II	$C_{25}H_{30}O_{14}$	553.1559	1.122	16147	57.74
2	PAB / 4-Aminobenzoic acid	$C_7H_7NO_2$	138.055	1.182	390972	87.82	Chlorogenic acid	$C_{16}H_{18}O_9$	353.0894	1.225	1277	82.2
3	cis-Sinapic acid	$C_{11}H_{12}O_5$	247.0573	1.327	13531	82.1	L-Malic acid	$C_4H_6O_5$	133.0144	1.225	2247	86.03
4	N-(1-Deoxy-1-fructosyl) phenylalanine	$C_{15}H_{21}NO_7$	328.1391	4.607	48920	81.07	2-Galloylglucose	$C_{13}H_{16}O_{10}$	331.0683	2.03	13713	85.45
5	2-Descarboxy-cyclo-dopa	$C_8H_9NO_2$	152.0705	4.329	86675	87.42	Gallic acid	$C_7H_6O_5$	169.0156	2.035	142553	78.82
6	Benzocaine	$C_9H_{11}NO_2$	166.0866	4.682	200367	87.19	Narcobarbital	$C_{11}H_{15}BrN_2O_3$	347.0241	2.294	16333	67.1
7	Isobutyl N- methyl anthranilate	$C_{12}H_{17}NO_2$	208.1336	5.106	67538	98.77	Ellagic acid	$C_{14}H_6O_8$	361.0205	2.832	2790	96.88
8	Tryptophyl-Valine	$C_{16}H_{21}N_3O_3$	326.1501	5.107	23055	66.47	Methyl 2-furoate	$C_6H_6O_3$	125.0255	2.838	141104	81.13
9	Indoleacrylic acid	$C_{11}H_9NO_2$	188.0714	5.418	694351	95.8	6'-Methoxy polygoacetophenoside	$C_{15}H_{20}O_{10}$	359.1023	5.149	109545	70.35
10	Euglobal-Ia1	$C_{23}H_{30}O_5$	409.1966	5.419	13420	79.82	DL-3,4-Dihydroxymandelic acid	$C_8H_8O_5$	183.0318	5.324	79483	84.91
11	Aspergillic acid	$C_{12}H_{20}N_2O_2$	247.145	5.43	474683	68.1	3-Hydroxynevirapine	$C_{15}H_{14}N_4O_2$	327.1122	6.131	18207	80.56
12	Mucronine B	$C_{28}H_{36}N_4O_4$	493.2839	5.484	738718	93.96	Canavalioside	$C_{26}H_{42}O_{12}$	545.2668	6.195	24243	61.55
13	N-Acetylserotonin	$C1_2H_{14}N_2O_2$	219.1133	5.771	148719	86.1	Dihydrocaffeic acid 3-O-glucuronide	$C_{15}H_{18}O_{10}$	403.0894	6.472	16862	95.88
14	6-Methylquinoline	$C_{10}H_9N$	144.0813	5.772	205633	86.51	Aprepitant	$C_{23}H_{21}F_7N_4O_3$	593.1587	6.695	11486	61.72
15	1-Naphthylamine	$C_{10}H_9N$	144.0815	6.174	235466	84.57	Unknown Comp. 1.17		643.1534	7.008	68521	-
16	Unknown Comp. 1.1		299.1402	6.063	91888	-	Pioglitazone	$C_{19}H_{20}N_2O_3S$	415.1306	7.255	11818	79.93
17	7-(Methylthio)hep tane-nitrile	$C_8H_{15}NS$	158.0972	6.288	240807	51.49	Tenitramine	$C_{10}H_{20}N_6O_{12}$	475.1323	7.305	95457	55.76
18	Unknown Comp. 1.2		299.1402	6.358	170070	-	Scleroglucan	$C_{24}H_{44}O_{20}P_2$	759.1884	7.366	15626	94.22
19	Biorobin	$C_{27}H_{30}O_{15}$	595.1675	6.656	151075	95.16	5-Amino-1-ribofuranosylimidazole-4-carboxyamide	$C_9H_{14}N_4O_6$	333.1031	8.632	40385	84.74
20	6-Cinnamoyl-1-galloylglucose	$C_{22}H_{22}O_{11}$	463.1247	6.721	50815	97.09	Unknown Comp. 1.18		635.2206	9.206	20310	-
21	Galangin 3-[galactosyl-(1->4)-	$C_{27}H_{30}O_{14}$	579.1723	6.806	96083	98.3	Urate-3- ribonucleoside	$C_{10}H_{12}N_4O_7$	299.0604	9.46	16017	58.63

Table 1. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
22	Chrysoeriol 7-O-neohe speridoside	$C_{28}H_{32}O_{15}$	609.1858	6.964	698075	96.92	Corchorifatty acid F	$C_{18}H_{32}O_5$	327.2225	9.511	23199	50.31
23	Unknown Comp. 1.3		357.0976	7.041	49275	-	Tragopogonsaponin K	$C_{50}H_{72}O_{15}$	971.4996	9.626	19470	95.62
24	Dimoracin	$C_{38}H_{32}O_8$	639.1933	7.305	42433	53.5	Ethyl 3,4,5-trimethoxybenzoate	$C_{12}H_{16}O_5$	239.096	9.922	18388	67.23
25	Galangin 3-[galactosyl-(1->4)-	$C_{27}H_{30}O_{14}$	579.1715	7.928	66205	98.43	9,10-Dihydroxy-12,13-epoxy octa decanoate	$C_{18}H_{34}O_5$	329.2376	10.494	12066	51.69
26	Retigabine	$C_{16}H_{18}FN_3O_2$	326.1297	8.041	146852	80.68	3-Deoxy-D-manno-octulosonate	$C_8H_{14}O_8$	283.0651	10.794	20728	74.3
27	Unknown Comp. 1.4		693.2402	8.961	132571	-	PIP (18:0/16:1(9Z))	$C_{43}H_{82}O_{16}P_2$	961.5092	11.605	137779	66.44
28	Unknown Comp. 1.5		618.2764	9.201	51250	-	9Z-Octa decenedioic acid	$C_{18}H_{32}O_4$	311.2274	11.855	44182	53.35
29	Epoxyganoderiol C	$C_{30}H_{48}O_3$	457.367	10.079	17628	97.47	Hoduloside VIII	$C_{46}H_{76}O_{18}$	961.5058	11.984	19499	63.3
30	Pyrohyperforin	$C_{35}H_{50}O_4$	557.3578	10.332	14848	61.72	PIP (18:1(9Z)/16:1(9Z))	$C_{43}H_{80}O_{16}P_2$	959.49	12.372	17033	71.11
31	Vignafuran	$C_{16}H_{14}O_4$	271.097	10.506	11583	93.99	Edulisin I	$C_{28}H_{26}O_8$	535.1623	13.297	210553	58.74
32	alpha,gamma-Onoceradienedione	$C_{30}H_{46}O_2$	439.3571	10.636	36275	98.25	Unknown Comp. 1.19		1035.3519	13.392	25144	-
33	1-(beta-D-Ribofuranosyl)-1,4-dihydro nicotinamide	$C_{11}H_{16}N_2O_5$	279.0941	10.786	10306	79.35	Methyl linoleate	$C_{19}H_{34}O_2$	339.2535	14.141	702	75.71
34	13-beta-D-Glucosyloxy docosanoate	$C_{28}H_{54}O_8$	541.3635	10.953	81137	33.38	α-Linolenic Acid	$C_{18}H_{30}O_2$	277.2212	16.76	144252	66.57
35	15-Oxo-21-hydroxymabiogenin 3- [rhamnosyl-(1->6)-glucoside]	$C_{42}H_{66}O_{15}$	811.4488	11.289	81704	97.75	Linalyl caprylate	$C_{18}H_{32}O_2$	279.2369	17.67	201260	65.5
36	xi-Tetrahydro-3-pentyl-2H-pyran-2-one	$C_{10}H_{18}O_2$	171.1385	11.582	12739	52.31	Calpeptin	$C_{20}H_{30}N_2O_4$	421.2322	18.245	76823	72.47
37	Chrysin dimethyl ether	$C_{17}H_{14}O_4$	283.0966	11.81	104203	99.91	Isopalmitic acid	$C_{16}H_{32}O_2$	255.237	18.472	264565	63.45
38	Panaxydol linoleate	$C_{35}H_{54}O_3$	545.3942	11.9	170467	88.21	4-Dodecylbenzenesulfonic acid	$C_{18}H_{30}O_3S$	325.1886	18.552	74882	63.9
39	Unknown Comp. 1.6		518.3682	12.343	79096	-	Unknown Comp. 1.20		281.2559	18.615	776516	-
40	Unknown Comp. 1.7		464.3365	12.768	45913	-	Pipercitine	$C_{23}H_{43}NO$	394.3392	18.692	179676	53.08

Table 1. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
41	Unknown Comp. 1.8		418.3148	12.971	15745	-	Imperialine	$C_{27}H_{43}NO_3$	428.3244	18.732	174440	53.51
42	Unknown Comp. 1.9		356.3155	12.983	143660	-	Unknown Comp. 1.21		281.2549	18.941	700123	-
43	Terminaline	$C_{23}H_{41}NO_2$	364.3203	13.121	53467	97.47						
44	Unknown Comp. 1.10	$C_{21}H_{20}O_6$	369.1314	13.204	2678	79.47						
45	Fluticasone propionate	$C_{25}H_{31}F_3O_5S$	501.1904	13.222	112829	94.89						
46	Unknown Comp. 1.11		366.3355	13.741	63187	-						
47	LysoPE(24:0/0:0)	$C_{29}H_{60}NO_7P$	566.4258	14.198	153661	57.31						
48	Unknown Comp. 1.12		368.3518	14.421	600513	14.733						
49	3-Ketosphinganine	$C_{18}H_{37}NO_2$	322.2733	14.996	70027	88.61						
50	Unknown Comp. 1.13		614.4742	15.204	12836	-						
51	Linoleoyl Ethanolamide	$C_{20}H_{37}NO_2$	324.2893	15.734	107567	96.43						
52	Taxa-4(20),11(12)-dien-5α,13α-diol	$C_{20}H_{32}O_2$	305.2474	15.886	86943	94.32						
53	plaunotol	$C_{20}H_{34}O_2$	307.2629	16.555	63913	95.79						
54	Oleoyl Ethanolamide	$C_{20}H_{39}NO_2$	326.3058	16.792	134733	99.83						
55	2alpha-(Hydroxy methyl)-5alpha-androstane-3beta,17beta-diol	$C_{20}H_{34}O_3$	323.258	17.096	163134	98.49						
56	Unknown Comp. 1.14		296.2946	17.774	92051	-						
57	Unknown Comp. 1.15		426.4304	18.161	11365	-						
58	Unknown Comp. 1.16		390.3008	18.37	172177	-						
59	Imperialine	$C_{27}H_{43}NO_3$	430.3314	18.438	62230	99.25						
60	Stearamide	$C_{18}H_{37}NO$	284.2954	18.605	11588	86.12						

Table 2. HRLCMS QTOF Compounds list of hydroalcoholic extract of classically processed *Abrus precatorius* L. red seeds

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
1	Anthranilic acid	$C_7H_7NO_2$	138.0538	1.516	305358	79.35	2-[(ethylthio)methyl] furan	$C_7H_{10}OS$	187.0435	1.311	42960	91.05
2	N-Acrylylglycine methyl ester	$C_6H_9NO_3$	144.0641	2.789	10537	72.69	2-Galloylglucose	$C_{13}H_{16}O_{10}$	331.0696	1.317	11729	71.59
3	Butethal	$C_{10}H_{16}N_2O_3$	235.1057	3.49	16116	95.26	Gallic acid	$C_7H_6O_5$	169.0159	2.055	86169	74.72
4	Laccarin	$C_{10}H_{14}N_2O_2$	217.0956	3.637	14613	91.12	Ellagic acid	$C_{14}H_6O_8$	361.0209	2.876	1035	81.46
5	2-Descarboxy-cyclo-dopa	$C_8H_9NO_2$	152.0693	4.305	58833	92.22	Unknown Comp. 2.14	$C_6H_{10}O$	143.0712	5.265	4342	83.24
6	Ketotifen	$C_{19}H_{19}NOS$	310.1264	4.457	38345	89.62	Canavalioside	$C_{26}H_{42}O_{12}$	545.2678	6.135	24257	56.15
7	Benzocaine	$C_9H_{11}NO_2$	166.0853	4.537	192078	81.54	Aprepitant	$C_{23}H_{21}F_7N_4O_3$	593.1591	6.686	11052	62.57
8	Butethal	$C_{10}H_{16}N_2O_3$	235.1059	4.593	65160	89.83	Unknown Comp. 2.15		643.1551	6.995	111914	-
9	Isobutyl N-methyl anthranilate	$C_{12}H_{17}NO_2$	208.1318	4.774	55051	87.96	6-beta-D- Glucopy ranosyl-4',5-dihydroxy-3',7-	$C_{23}H_{24}O_{11}$	475.1333	7.251	212084	52
10	N-Acetylserotonin	$C_{12}H_{14}N_2O_2$	219.1122	5.085	544564	96.05	Tenitramine	$C_{10}H_{20}N_6O_{12}$	475.1324	7.603	52174	54.92
11	Indoleacrylic acid	$C_{11}H_9NO_2$	188.0701	5.087	522237	96.84	3-Deoxy-D-manno-octulosonate	$C_8H_{14}O_8$	283.0663	10.774	26246	90.38
12	Isocarbostyril	C_9H_7NO	146.059	5.171	142586	82.24	Phytolaccoside D2	$C_{42}H_{66}O_{15}$	809.4467	11.295	36223	51.62
13	p-Aminobenzamidine	$C_7H_9N_3$	158.0695	5.249	13709	45.49	Fungichromin	$C_{35}H_{58}O_{12}$	669.3889	11.51	12896	62.41
14	Aspergillic acid	$C_{12}H_{20}N_2O_2$	247.1431	5.378	306549	89.98	PIP (18:0/16:1(9Z))	$C_{43}H_{82}O_{16}P_2$	961.5121	11.585	201884	56.05
15	Erinacine P	$C_{27}H_{40}O_8$	493.2795	5.432	687453	78.28	TR-Saponin B	$C_{52}H_{80}O_{20}$	1023.51	11.627	14118	68.95
16	Primidone	$C_{12}H_{14}N_2O_2$	219.1116	5.446	139509	93.63	Octadecanedioic acid	$C_{18}H_{34}O_4$	313.2436	12.384	13943	58.87
17	Fulvine	$C_{16}H_{23}NO_5$	310.1636	5.795	496787	93.78	MG (15:0/0:0/0:0)	$C_{18}H_{36}O_4$	315.2588	13.506	18116	61.64
18	Samin	$C_{13}H_{14}O_5$	251.09	5.798	151779	92.53	Sambutoxin	$C_{28}H_{39}NO_4$	452.2848	13.543	12720	67.85
19	L-phenylalanyl-L-hydroxyproline	$C_{14}H_{18}N_2O_4$	301.1165	6.021	123572	97	3,6-Epoxy-5,5',6,6'-tetrahydro-b, b-carotene-3',5,5',6'-tetrol	$C_{40}H_{58}O_5$	617.4147	13.912	11011	56.57
20	6-Methylquinoline	$C_{10}H_9N$	144.0805	6.094	623763	83.26	Pederin	$C_{25}H_{45}NO_9$	562.3232	14.273	11661	99.3

Table 2. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
21	3-Butylpyridine	$C_9H_{13}N$	158.0958	6.15	213706	70.26	Unknown Comp. 2.16		640.3562	14.772	13725	-
22	3-Hydroxymono ethylglycylxylidide (3-Hydroxy-MEGX)	$C_{12}H_{18}N_2O_2$	245.1271	6.26	164197	80.6	Sambutoxin	$C_{28}H_{39}NO_4$	452.285	14.997	11437	65.18
23	Kuwanon Z	$C_{34}H_{26}O_{10}$	595.1615	6.681	102722	89.91	3-keto stearic acid	$C_{18}H_{34}O_3$	297.2481	15.033	13436	61.88
24	Reduced pyocyanine	$C_{13}H_{12}N_2O$	213.1015	6.762	20653	91.48	3-Hydroxy-beta-ionol 3-[glucosyl-(1->6)-glucoside]	$C_{25}H_{42}O_{12}$	593.2826	15.177	45022	95.83
25	Ginkgolide C	$C_{20}H_{24}O_{11}$	463.12	6.763	67506	96.01	5-Oxoavermectin ‘‘1a” aglycone	$C_{34}H_{46}O_8$	641.3413	15.264	14055	29.72
26	7-Dehydrologanin tetraacetate	$C_{25}H_{32}O_{14}$	579.1668	6.851	95138	95.9	Mifepristone	$C_{29}H_{35}NO_2$	474.2694	15.913	14240	62.25
27	Calendoflaside	$C_{28}H_{32}O_{15}$	609.1792	6.991	765910	78.02	Gymnodimine	$C_{32}H_{45}NO_4$	566.3547	16.502	22069	59.03
28	Phlorhizin	$C_{21}H_{24}O_{10}$	459.1251	7.074	32297	94	LysoPE(0:0/18:0)	$C_{23}H_{48}NO_7P$	540.3389	16.537	19853	53.63
29	6-Methylquinoline	$C_{10}H_9N$	144.1799	7.455	79403	82.5	Psychosine	$C_{24}H_{47}NO_7$	506.3325	16.588	11369	95.57
30	Neocarzinostatin chromophore	$C_{35}H_{33}NO_{12}$	681.198	7.512	54839	51.66	α-Linolenic Acid	$C_{18}H_{30}O_2$	277.2219	16.753	151378	61.16
31	Unknown Comp. 2.1		681.1978	7.801	176463	-	Auriculine	$C_{31}H_{45}NO_8$	618.3269	16.853	21532	86.49
32	Evodiamine	$C_{19}H_{17}N_3O$	326.1268	8.026	118360	89.01	LysoPE(0:0/20:1(11Z))	$C_{25}H_{50}NO_7P$	566.3553	16.897	98430	51.86
33	Kuwanone G	$C_{40}H_{36}O_{11}$	693.2344	8.904	40381	90.36	Medicagenic acid beta-maltoside	$C_{42}H_{66}O_{16}$	871.4239	17.577	11286	55.33
34	Unknown Comp. 2.2		618.2716	9.049	41397	-	Linalyl caprylate	$C_{18}H_{32}O_2$	279.2371	17.661	116835	61.14
35	Prunetin	$C_{16}H_{12}O_5$	285.0747	10.637	62913	94.62	Isopalmitic acid	$C_{16}H_{32}O_2$	255.2372	18.474	189724	61.85
36	15-Oxo-21-hydroxymabiogenin 3- [rhamnosyl-(1->6)-glucoside]	$C_{42}H_{66}O_{15}$	811.444	11.472	84211	86.34	Unknown Comp. 2.17		402.3066	18.596	15238	-
37	Veratramine	$C_{27}H_{39}NO_2$	432.2942	11.749	46871	55.21	Unknown Comp. 2.18		281.2559	18.615	782151	-
38	(S)-Auraptenol	$C_{15}H_{16}O_4$	283.095	11.813	106644	96.02	Pipercitine	$C_{23}H_{43}NO$	394.3393	18.662	156898	54.13
39	Panaxydol linoleate	$C_{35}H_{54}O_3$	545.3913	11.988	105505	63.29	Hydroquinidine	$C_{20}H_{26}N_2O_2$	325.1895	18.692	102106	68.33

Table 2. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
40	Unknown Comp. 2.3		518.3648	12.077	44141	-	Imperialine	$C_{27}H_{43}NO_3$	428.3247	18.737	147142	53.23
41	Ganoderiol I	$C_{31}H_{50}O_5$	525.3648	12.601	34524	0.78	Unknown Comp. 2.19		281.2546	18.964	596179	-
42	Unknown Comp. 2.4		356.3133	12.689	103757	-	MG (18:2(9Z,12Z)/0:0/0:0) [ra	$C_{21}H_{38}O_4$	353.2762	19.23	162530	54.67
43	Retapamulin	$C_{30}H_{47}NO_4S$	518.3205	14.195	161968	48.33	Petroselinic acid	$C_{18}H_{34}O_2$	281.2536	19.333	134640	59.09
44	Unknown Comp. 2.5		368.3503	14.418	303384	-	14,19-Dihydroaspidospermatine	$C_{21}H_{28}N_2O_2$	339.2052	19.776	54202	74.66
45	(3a,5b,7a,12a)-24-[(carboxymethyl) amino]-1,12-dihydroxy-24-oxocholan-3-yl-b-D-Glucopyranosiduronic a	$C_{32}H_{51}NO_{12}$	642.3565	14.645	69374	55.46						
46	Unknown Comp. 2.6		520.3357	14.855	120219	-						
47	23-Acetoxy soladulcidine	$C_{29}H_{47}NO_4$	496.3368	15.735	180181	76.19						
48	Mycinamicin VII	$C_{29}H_{47}NO_7$	522.3524	16.201	783696	52.52						
49	Unknown Comp. 2.7		522.3542	16.551	1165524	-						
50	Unknown Comp. 2.8		504.3411	16.61	13109	-						
51	Unknown Comp. 2.9		594.3734	17.117	21781	-						
52	Acetylgitaloxin	$C_{44}H_{66}O_{16}$	873.4231	17.471	86037	98.14						
53	Unknown Comp. 2.10		296.2936	17.774	94187	-						
54	Unknown Comp. 2.11		512.5006	17.829	44533	-						
55	Unknown Comp. 2.12		816.6519	18.851	10440	-						
56	Unknown Comp. 2.13		458.3598	19.476	33755	-						

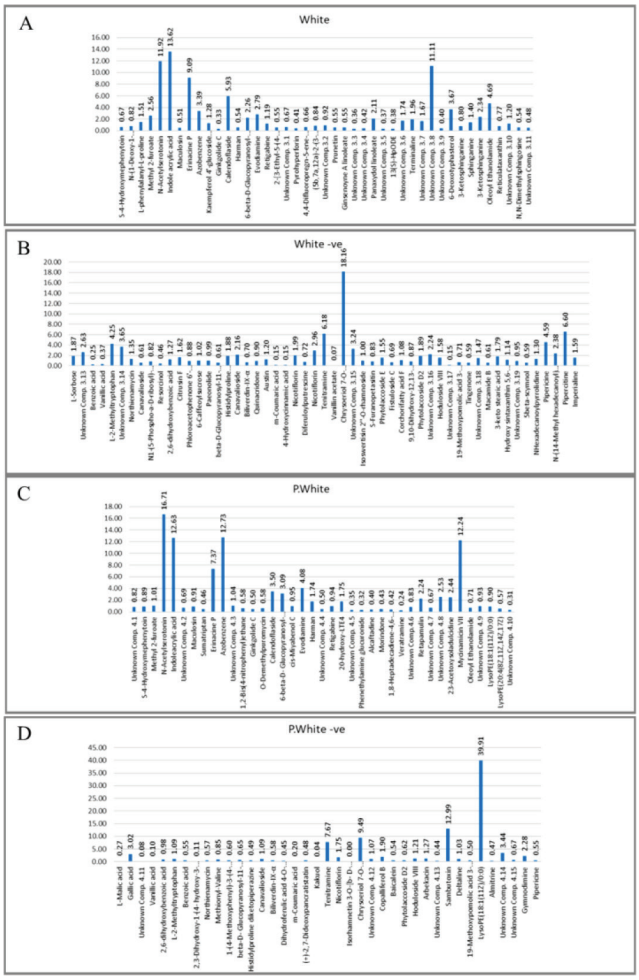


Figure 3. Percentage areas of various metabolites present in hydroalcoholic extracts of unprocessed and processed *Abrus precatorius* L. white seeds. **(A)** White seed extract (positive ion mode), **(B)** White seed extract (negative ion mode), **(C)** Processed White seed extract (positive ion mode) and D-Processed White seed extract (negative ion mode).

Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone, Scoparin 2"-glucoside and cis-Miyabenol C in the processed black seed extract.

These metabolites were organised in the order of higher affinity to lower affinity and the interaction patterns were analysed. It reveals that various docking poses of the higher active molecules and the Pallidol 3-glucoside present in the hydroalcoholic extract of black seeds have shown a higher active score value (-7.91946) and the docking pose of this is compared with the standard ligand rociletinib with the score value of (-4.35987) as shown in Figure 6. The interaction diagrams of other top active molecules are given in Figure 7.

Other than the general interaction with the amino acids, hydrogen bonds are formed between the metabolites and the target site. The hydrogen bond formations are expressed in Figures 6 and 7. Pallidol 3-glucoside forms six hydrogen bonds with various amino acids of the target site such as Leu718, Met793, Pro794, Asp800, Arg841, and Asp855. By ellagic acid, two hydrogen bonds are formed with Met793 and the other two with Asp855. 6'-Methoxy polygoacetophenoside was found to be the third metabolite with a higher active gscore value which forms four hydrogen bonds with various amino acids of the target site such as Asp855 and Met793. Out of the four, 3 bonds were formed with Asp555. Chrysoeriol 7-O-neohesperidoside forms three hydrogen bonds with Glu804, one hydrogen bond with Asp800, one hydrogen bond with Phe795, one hydrogen bond with Met793 and two with Lys745 and Asp855. 6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone makes one hydrogen bond with Met793, two hydrogen bonds one with Lys745 and one with Asp855. Scoparin 2'-glucoside formed one hydrogen bond each with Arg841, Asp800, Thr854, Asp855, and Gly724 and two bonds with Met793. A total of three hydrogen bonds are formed by cis-Miyabenol C, one each with Gln791, Thr954 and Asp855. A total of four hydrogen bonds are formed by PIP (18:0/16:1(9Z)), one with Asp855, Asn842 and two with Asp800. A total of seven hydrogen bonds with various amino acids was formed by Phlorhizin, one each with Pro794, Met793, Gln791, Lys 745 and three bonds with Asp855. Phloroacetophenone 6'-[xylosyl-(1->6)-glucoside] forms a total of eight hydrogen bonds are formed, one each with Met793, Cys797, Lys745 and two bonds with Asp 855and three bonds with Asp800. Paeonolide forms nine bonds in total. One each with Met793, Cys797, Lys745, Phr854, two bonds with Asp855 and three bonds with Asp800. 2-[3-Ethyl-5-(4-methoxyphenyl)-1H-pyrazol-4-yl] phenol forms three hydrogen bonds, one each with Thr854, Gln791 and Met793. Biorobin forms eight hydrogen bonds in total. One each with Met793 and Thr854, two bonds with Lys745, and 4 bonds with Asp855. Nicotiflorin forms eight hydrogen bonds in total. One each with Met793 and Thr854, two bonds with Lys745, and 4 bonds with Asp855. Five hydrogen bonds in total are formed by Biliverdin-IX-α, one each with Ser720, Lys754, and Thr854, and two bonds with Asp855. Isocarbostyril forms two hydrogen bonds one each with Met793 and Gln 791. Isorhamnetin 3-O- [b- D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside] forms five hydrogen bonds one each with Leu718, Gln791, Lys745, Arg841, Asn842.

Table 3. HRLCMS QTOF Compounds list of hydroalcoholic extract of *Abrus precatorius* L. white seeds

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
1	S-4-Hydroxy mephenytoin	$C_{12}H_{14}N_2O_3$	235.1068	1.802	193407	96.51	Unknown Comp. 3.12	$C_8H_{10}N_4O_2$	253.0925	0.969	878	72.01
2	N-(1-Deoxy-1-fructosyl) phenylalanine	$C_{15}H_{21}NO_7$	328.1374	2.034	244085	91.42	L-Sorbose	$C_6H_{12}O_6$	179.0563	1.057	249514	99.54
3	L-phenylalanyl-L-proline	$C_{14}H_{18}N_2O_3$	263.1381	2.494	318930	96.44	Unknown Comp. 3.13	$C_4H_6O_5$	133.0145	1.191	17806	87.02
4	Methyl 2-furoate	$C_6H_6O_3$	127.0388	2.731	1887869	87.59	Benzoic acid	$C_7H_6O_2$	121.0301	2.521	399	74.66
5	N-Acetylserotonin	$C_{12}H_{14}N_2O_2$	219.1121	3.006	2493712	96.88	Vanillic acid	$C_8H_8O_4$	167.0354	2.521	2177	71.87
6	Indole acrylic acid	$C_{11}H_9NO_2$	188.0702	3.041	1667741	86.62	L-2-Methyltryptophan	$C_{12}H_{14}N_2O_2$	217.0996	3.063	641884	91.78
7	Maculosin	$C_{14}H_{16}N_2O_3$	261.1221	3.304	87367	81	Unknown Comp. 3.14		507.1398	3.319	277181	-
8	Erinacine P	$C_{27}H_{40}O_8$	493.2778	3.785	2065364	92.57	Northienamycin	$C_{10}H_{14}N_2O_4S$	303.0647	3.576	237515	87.59
9	Azobenzene	$C_{12}H_{10}N_2$	183.0913	4.494	481430	99.74	Canavalioside	$C_{26}H_{42}O_{12}$	545.2643	3.581	138370	78.56
10	Kaempferol 4'-glucoside 7-rhamnoside	$C_{27}H_{30}O_{15}$	595.1624	5.44	132978	85.04	N1-(5-Phospho-a-D-ribosyl)-5,6-dimethyl benzimidazole	$C_{14}H_{19}N_2O_7P$	417.1072	3.796	121875	98.24
11	Ginkgolide C	$C_{20}H_{24}O_{11}$	463.1209	5.727	125509	99.35	Resorcinol	$C_6H_6O_2$	109.03	4.008	5977	76.91
12	Calendoflaside	$C_{28}H_{32}O_{15}$	609.1775	5.946	674359	85.14	2,6-dihydroxybenzoic acid	$C_7H_6O_4$	153.0201	4.008	18083	95.98
13	Harman	$C_{12}H_{10}N_2$	183.0912	5.982	187227	98.62	Citrusin F	$C_{22}H_{32}O_{14}$	519.1774	4.118	244786	66.65
14	6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone	$C_{23}H_{24}O_{11}$	477.1364	6.469	487469	85.67	Phloroacetophenone 6'-[xylosyl-(1->6)-glucoside]	$C_{21}H_{30}O_{13}$	489.1655	4.274	135678	73.52
15	Evodiamine	$C_{19}H_{17}N_3O$	326.1273	6.813	382386	78.49	6-Caffeoylsucrose	$C_{21}H_{28}O_{14}$	563.1665	4.36	95155	70.21
16	Retigabine	$C_{16}H_{18}FN_3O_2$	326.1273	7.419	278059	80.09	Paeonolide	$C_{20}H_{28}O_{12}$	459.1551	4.571	183792	72.52
17	2-[3-Ethyl-5-(4-methoxyphenyl)-1H-pyrazol-4-yl] phenol	$C_{18}H_{18}N_2O_2$	317.1273	7.449	158380	92.92	beta-D-Glucopyranosyl-11-hydroxy jasmonic acid	$C_{18}H_{28}O_9$	387.1694	4.641	94003	55.17

Table 3. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
18	Unknown Comp. 3.1		432.2724	8.846	286113	-	Histidylproline diketopiperazine	$C_{12}H_{16}N_4O_2$	307.1431	4.916	504024	83.74
19	Pyrohyperforin	$C_{35}H_{50}O_4$	557.3551	8.92	135000	51.02	Canavalioside	$C_{26}H_{42}O_{12}$	545.266	5.06	265409	65.82
20	4,4-Difluoropregn-5-ene-3,20-dione	$C_{21}H_{28}F_2O_2$	351.2126	9.362	578869	93.16	Biliverdin-IX-α	$C_{33}H_{34}N_4O_6$	581.2423	5.063	138461	63.68
21	(5b,7a,12a)-2-(3-methoxyphenyl)-2-oxoethyl ester-7,12-dihydroxy-cholan-24-oic acid	$C_{33}H_{48}O_6$	541.3605	9.728	285826	55.85	Quinacridone	$C_{20}H_{12}N_2O_2$	371.102	5.203	194662	76.39
22	Unknown Comp.3.2		436.3031	9.947	473091	-	Austin	$C_{27}H_{32}O_9$	499.2001	5.363	158249	61.71
23	Prunetin	$C_{16}H_{12}O_5$	285.0743	10.01	136640	91.97	m-Coumaric acid	$C_9H_8O_3$	163.041	5.401	1343	77.51
24	Ginsenoyne A linoleate	$C_{35}H_{52}O_3$	543.3759	10.232	242786	63.81	4-Hydroxycinnamic acid	$C_9H_8O_3$	163.041	5.401	1343	77.51
25	Unknown Comp. 3.3		478.3341	10.511	49651	-	Nicotiflorin	$C_{27}H_{30}O_{15}$	593.1565	5.446	85576	62
26	Unknown Comp. 3.4		316.2829	10.578	176647	-	Diferuloylputrescine	$C_{24}H_{28}N_2O_6$	439.1864	5.487	91486	83.56
27	Panaxydol linoleate	$C_{35}H_{54}O_3$	545.3912	10.726	726852	63.93	Nicotiflorin	$C_{27}H_{30}O_{15}$	593.1575	5.768	532476	64.31
28	Unknown Comp. 3.5		518.3651	10.813	129614	-	Tenitramine	$C_{10}H_{20}N_6O_{12}$	461.1139	5.769	250353	81.63
29	13(S)-HpODE	$C_{18}H_{32}O_4$	335.2175	11.3	307966	89.5	Vanillin acetate	$C_{10}H_{10}O_4$	193.0517	5.886	581	70.78
30	Unknown Comp. 3.6		356.3139	11.513	378456	-	Chrysoeriol 7-O-neohesperidoside	$C_{28}H_{32}O_{15}$	607.1729	5.97	2028943	65.92
31	Terminaline	$C_{23}H_{41}NO_2$	364.3189	11.853	517167	88.39	Unknown Comp. 3.15		643.1501	5.971	302211	-
32	Unknown Comp. 3.7		366.3348	12.543	343981	-	Isoswertisin 2”-O-rhamnoside	$C_{28}H_{32}O_{14}$	637.1836	6.312	119040	64.22
33	Unknown Comp. 3.8		368.3503	13.188	593917	-	S-Furanopetasitin	$C_{24}H_{32}O_5S$	491.218	7.613	114719	45.68
34	Unknown Comp. 3.9		396.3565	13.783	1900554	-	Phytolaccoside E	$C_{42}H_{66}O_{16}$	825.4349	7.77	1642777	66.46
35	6-Deoxotyphasterol	$C_{28}H_{50}O_3$	457.365	13.846	336743	98.36	Fistuloside C	$C_{45}H_{72}O_{19}$	975.4806	9.359	149454	69.08

Table 3. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
36	3-Ketosphinganine	$C_{18}H_{37}NO_2$	322.2727	14.435	271730	94.38	Corchorifatty acid F	$C_{18}H_{32}O_5$	327.2215	9.429	469697	58.49
37	Sphinganine	$C_{18}H_{39}NO_2$	324.2884	15.34	198609	98.1	9,10-Dihydroxy-12,13-epoxyoctadecanoate	$C_{18}H_{34}O_5$	329.2366	9.734	113895	73.41
38	3-Ketosphinganine	$C_{18}H_{37}NO_2$	300.288	16.188	266321	95.15	Phytolaccoside D2	$C_{42}H_{66}O_{15}$	809.4408	10.749	265357	63.79
39	Oleoyl Ethanolamide	$C_{20}H_{39}NO_2$	326.3037	16.523	1558172	92.15	Unknown Comp. 3.16		961.5016	11.126	323521	-
40	Reticulataxanthin	$C_{33}H_{44}O_2$	495.3259	17.45	223409	72.5	Hoduloside VIII	$C_{46}H_{76}O_{18}$	961.5017	11.276	1165802	68.54
41	Unknown Comp. 3.10		296.2935	17.662	416663	-	Unknown Comp. 3.17	$C_{18}H_{28}O_3$	351.2181	11.897	882	81.22
42	N, N-Dimethyl sphingosine	$C_{20}H_{41}NO_2$	328.3194	17.965	292070	91.5	19-Methoxypomolic acid 3-arabinoside	$C_{36}H_{58}O_8$	617.4113	13.855	147253	68.74
43	Unknown Comp. 3.11	$C_{35}H_{50}O_4$	390.2977	18.591	174614	-	Tingenone	$C_{28}H_{36}O_3$	479.2821	16.373	212865	63.09
44							Unknown Comp. 3.18		410.2952	16.594	301552	-
45							Macamide B	$C_{23}H_{39}NO$	390.305	16.665	128075	70.02
46							3-keto stearic acid	$C_{18}H_{34}O_3$	297.2463	17.283	380561	78.91
47							Hydroxy sintaxanthin 5,6-epoxide	$C_{31}H_{42}O_3$	507.3145	17.822	694076	61.37
48							Unknown Comp. 3.19		426.3054	18.048	170102	-
49							5beta-scymnol	$C_{27}H_{48}O_6$	467.3326	18.193	129283	63.5
50							N-Hexadecan oylpyrrolidine	$C_{20}H_{39}NO$	354.3048	18.292	292665	71.44
51							Pipericine	$C_{22}H_{41}NO$	380.3209	18.386	1003665	68.65
52							N-(14-Methyl hexadecanoyl) pyrrolidine	$C_{21}H_{41}NO$	368.3211	18.539	382660	66.9
53							Pipercitine	$C_{23}H_{43}NO$	394.337	18.743	1096999	65.21
54							Imperialine	$C_{27}H_{43}NO_3$	428.3207	19.224	132787	70.65

Table 4. HRLCMS QTOF Compounds list of hydroalcoholic extract of classically processed *Abrus precatorius* L. white seeds

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
1	Unknown Comp. 4.1		120.0806	1.712	467631	-	L-Malic acid	$C_4H_6O_5$	133.0148	1.258	2333	83.68
2	S-4-Hydroxymephenytoin	$C_{12}H_{14}N_2O_3$	235.107	1.779	228098	98.05	Gallic acid	$C_7H_6O_5$	169.0149	1.612	43286	97.69
3	Methyl 2-furoate	$C_6H_6O_3$	127.0388	2.79	579578	87.57	Unknown Comp. 4.11	$C_6H_6O_2$	155.0354	2.088	1135	78.93
4	N-Acetylserotonin	$C_{12}H_{14}N_2O_2$	219.112	3.118	1045950	96.29	Vanillic acid	$C_8H_8O_4$	167.0354	2.517	1416	77.58
5	Indoleacrylic acid	$C_{11}H_9NO_2$	188.0702	3.119	971298	86.17	2,6-dihydroxybenzoic acid	$C_7H_6O_4$	153.0199	2.811	5258	85.7
6	Unknown Comp. 4.2		542.2459	3.182	94681	-	L-2-Methyltryptophan	$C_{12}H_{14}N_2O_2$	217.0997	3.165	248173	79.25
7	Maculosin	$C_{14}H_{16}N_2O_3$	261.1234	3.308	93465	85.68	Benzoic acid	$C_7H_6O_2$	181.0511	3.254	12658	92.9
8	Sumatriptan	$C_{14}H_{21}N_3O_2S$	296.1478	3.447	89040	51.28	2,3-Dihydroxy-1-(4- hydroxy-3-methoxyphenyl)-1-propanone	$C_{10}H_{12}O_5$	211.0613	3.686	435	70.37
9	Erinacine P	$C_{27}H_{40}O_8$	493.278	3.835	2645550	91.67	Northienamycin	$C_{10}H_{14}N_2O_4S$	303.0641	3.754	93967	84.18
10	Azobenzene	$C_{12}H_{10}N_2$	183.0915	4.42	276211	96.54	Methionyl-Valine	$C_{10}H_20N_2O_3S$	293.1171	3.835	215759	91.89
11	Unknown Comp. 4.3		476.2252	4.45	302811	-	1-(4-Methoxyphenyl)-3-(4-morpholinyl)-1-propanone	$C_{14}H_{19}NO_3$	294.1366	4.264	95056	86.7
12	1,2-Bis(4-nitrophenyl) ethane	$C_{14}H_{12}N_2O_4$	273.0862	4.567	137988	97.67	beta-D-Glucopyranosyl-11-hydroxy jasmonic acid	$C_{18}H_{28}O_9$	387.1692	4.673	108066	71.05
13	Ginkgolide C	$C_{20}H_{24}O_{11}$	463.121	5.775	146698	99.55	Histidylproline diketopiperazine	$C_{12}H_{16}N_4O_2$	307.1423	4.894	90209	92.67
14	O-Demethyl puromycin	$C_{21}H_{27}N_7O_5$	458.2148	5.783	166447	98.5	Canavalioside	$C_{26}H_{42}O_{12}$	545.2647	5.055	202622	75.59
15	Calendoflaside	$C_{28}H_{32}O_{15}$	609.1776	6.023	148227	81.32	Biliverdin-IX-α	$C_{33}H_{34}N_4O_6$	581.2413	5.057	165495	60.84
16	6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone	$C_{23}H_{24}O_{11}$	477.1361	6.063	526258	88.72	Dihydroferulic acid 4-O-glucuronide	$C_{16}H_{20}O_{10}$	371.1013	5.197	118138	80.44

Table 4. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
17	cis-Miyabenol C	$C_{42}H_{32}O_9$	681.1989	6.441	156701	43.51	m-Coumaric acid	$C_9H_8O_3$	163.0402	5.327	2505	81.85
18	Evodiamine	$C_{19}H_{17}N_3O$	326.1275	6.812	269465	85.35	(+)-2,7-Dideoxy pancratistatin	$C_{14}H_{15}NO_6$	292.0847	5.599	69499	85.39
19	Harman	$C_{12}H_{10}N_2$	183.0912	6.972	252338	85.55	Kakuol	$C_{10}H_{10}O_4$	193.0512	5.729	2321	77.44
20	Unknown Comp. 4.4		682.2816	7.006	120065	-	Tenitramine	$C_{10}H_{20}N_6O_{12}$	461.1127	5.753	216676	87.18
21	Retigabine	$C_{16}H_{18}FN_3O_2$	326.1274	7.144	398866	85.45	Nicotiflorin	$C_{27}H_{30}O_{15}$	593.1561	5.754	299426	73.35
22	20-hydroxy-LTE4	$C_{23}H_{37}NO_6S$	478.231	7.307	284298	46.45	Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	$C_{28}H_{32}O_{16}$	623.1659	5.829	157200	78.73
23	Unknown Comp. 4.5		450.1996	7.335	133424	-	Chrysoeriol 7-O-neohesperidoside	$C_{28}H_{32}O_{15}$	607.1724	5.974	93939	66.67
24	Phenethylamine glucuronide	$C_{14}H_{19}NO_6$	298.1324	7.338	90865	36.08	Unknown Comp. 4.12		643.1492	5.976	238082	
25	Alcaftadine	$C_{19}H_{21}N_3O$	330.1585	8.216	76765	91.91	Copalliferol B	$C_{42}H_{32}O_9$	679.1939	6.387	177578	66.58
26	Morindone	$C_{15}H_{10}O_5$	271.0591	8.522	70199	95.93	Baicalein	$C_{15}H_{10}O_5$	269.0483	8.535	2751	74.72
27	1,8-Heptadecadiene-4,6-diyne-3,10-diol	$C_{17}H_{24}O_2$	261.184	10.155	80425	96.23	Phytolaccoside D2	$C_{42}H_{66}O_{15}$	809.4412	10.876	304259	61.57
28	Veratramine	$C_{27}H_{39}NO_2$	432.2941	11.109	75686	54.9	Hoduloside VIII	$C_{46}H_{76}O_{18}$	961.5017	11.329	1104755	66.64
29	Unknown Comp.4.6		356.3137	11.555	136782	-	Arbekacin	$C_{22}H_{44}N_6O_{10}$	597.3104	12.709	161403	99.17
30	Retapamulin	$C_{30}H_{47}NO_4S$	518.3211	13.603	948049	44.03	Unknown Comp. 4.13	$C_{18}H_{30}O_3$	353.2317	12.917	1845	75.22
31	Unknown Comp. 4.7		368.3503	13.678	162373	-	Sambutoxin	$C_{28}H_{39}NO_4$	452.2829	13.577	480340	76.02
32	Unknown Comp. 4.8		520.3365	14.669	550191	-	Deltaline	$C_{27}H_{41}NO_8$	552.2912	13.668	190340	19.42
33	23-Acetoxys oladulcidine	$C_{29}H_{47}NO_4$	496.3363	15.39	111303	80.6	19-Methoxypomolic acid 3-arabinoside	$C_{36}H_{58}O_8$	617.4116	13.799	103041	66.71
34	Mycinamicin VII	$C_{29}H_{47}NO_7$	522.3523	15.692	318060	50.1	LysoPE(18:1(11Z)/0:0)	$C_{23}H_{46}N\ O_7P$	478.2988	14.804	522761	68.12
35	Oleoyl Ethanolamide	$C_{20}H_{39}NO_2$	326.3037	16.581	191168	91.34	Almitrine	$C_{26}H_{29}F_2N_7$	536.2569	15.543	90154	38.03
36	Unknown Comp. 4.9		296.2935	17.715	208182	-	Unknown Comp. 4.14		556.3227	15.789	83171	-
37	LysoPE(18:1(11Z)/0:0)	$C_{23}H_{46}NO_7P$	502.2876	18.34	212363	84.73	Unknown Comp. 4.15		530.3064	15.84	95505	-
38	LysoPE(20:4 (8Z,11Z,14Z,17Z)	$C_{25}H_{44}NO_7P$	524.2692	18.418	99583	63.97	Gymnodimine	$C_{32}H_{45}NO_4$	506.3301	16.193	199999	78.27
39	Unknown Comp. 4.10		396.3448	18.853	126391	-	Pipericine	$C_{22}H_{41}NO$	380.3207	18.48	193224	70.26

Calendoflaside forms five hydrogen bonds in total one each with Cys797, Asp800, Asp855 and two with Arg841. Indole acrylic acid forms four hydrogen bonds in total one each with Lys745, Gln791, Glu762, and Asp855. Finally, Prunetin forms three hydrogen bonds, each with Met793, Lys754, and Asp855.

4. Discussion

The seeds of *Abrus precatorius* were reported for the numerous phytoconstituents. It is rich in several amino acids such as abrusin, serine, alanine, trimethyl, tryptophan, kiakasaponin III, sophoradiol, ursolic acid, valine, amyrine etc. It is famous for its toxic protablumin named abrine and its different types such as abrin A, abrin B, Abrin c, Abrin 1, Abrin II, Abrin III, Abrus saponin I and II and Abris Apogenol. It has other phytoconstituents such as eicos-11-enoic acid, hexadecenoic acid, octadecane, octanoic acid, nonacosane, hypaphorine, trigonelline, choline, abrisin, squalene etc[22].

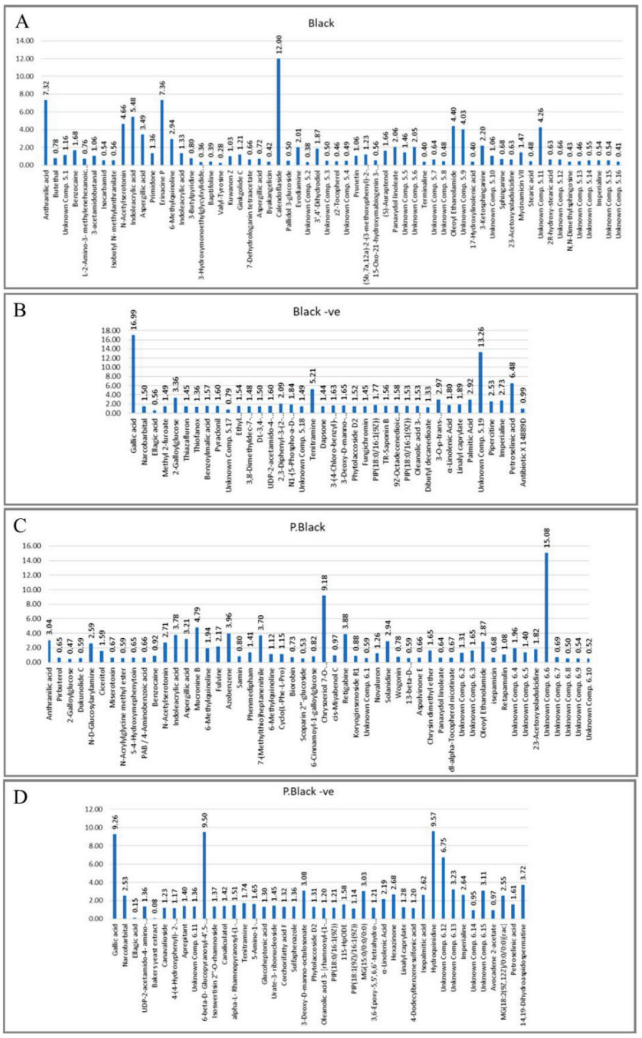


Figure 4. Percentage areas of various metabolites present in hydroalcoholic extracts of unprocessed and processed *Abrus precatorius* L. black seeds. **(A)** Black seed extract (positive ion mode), **(B)** Black seed extract (negative ion mode), **(C)** Processed black seed extract (positive ion mode) and **(D)** Processed black seed extract (negative ion mode).

Epidermal growth factor is an important polypeptide produced in the human body with 53 amino acid residues that play a vital role in cell proliferation. It exerts its biological activity by acting through a transmembrane protein tyrosine kinase which is widely called an Epidermal Growth Factor Receptor (EGFR)[23]. The human EGF receptor (EGFR) is a transmembrane glycoprotein of 1186 amino acid length belonging to the tyrosine kinase family[24]. The epidermal growth factor acts by binding to the 622 amino acid length extracellular amino terminal of the Epidermal Growth Factor Receptor. It is divided into domains I to IV which are named L1, S1, L2 and S2 respectively. Thirty-seven per cent of the identity of amino acids is shared by domains I and III, whereas the other two domains II and IV are homologous and rich in amino acid Cysteine (CR1 and CR2)[25,26]. In an ordinary cell, EGFR plays an important role in triggering two main signalling pathways.

Hence, EGFR is considered a vital factor in various disorders. Any abnormalities related to EGFR, or the pathways related to it may lead to the pathogenesis of several disorders such as breast cancer, ovarian cancer, non-small cell lung carcinoma, oesophageal, colorectal cancer etc. This receptor is involved in many tumour generation signalling pathways and hence it plays an important role in the development of resistance to chemotherapy and radiation therapy[27]. It is more expressed up to 30-89 % in pancreatic ductal cancer patients[28]. In certain cases, the activation of EGFR will lead to various inflammatory diseases and skin disorders such as dermatitis, psoriasis etc. On the other hand, inhibition of EGFR by tyrosine kinase inhibitors and monoclonal antibodies may lead to monomorphic acne form reactions. In kidneys, EGFR expressed in the glomerulus and tubulointerstitial compartment plays a vital role in renal physiology such as homeostasis of renal electrolytes. The upregulation of EGFR pathways in kidneys may lead to various disorders such as glomerulonephritis, polycystic kidney disorders, diabetic nephropathy, and rejection of transplants. By having an overall view, it can be understandable that any molecule that can act on EGFR may result in different

Table 5. HRLCMS QTOF Compounds list of hydroalcoholic extract of *Abrus precatorius* L. black seeds

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
1	Anthranilic acid	$C_7H_7NO_2$	138.0538	1.502	672403	81.89	Gallic acid	$C_7H_6O_5$	169.0157	2.038	131204	89.74
2	Butethal	$C_{10}H_{16}N_2O_3$	235.1059	3.541	13649	78.1	Narcobarbital	$C_{11}H_{15}BrN_2O_3$	347.0254	2.71	31048	68.17
3	Unknown Comp. 5.1		120.0801	3.648	11572	-	Ellagic acid	$C_{14}H_6O_8$	361.0208	2.863	2684	97.7
4	Benzocaine	$C_9H_{11}NO_2$	166.0852	3.868	11133	91.45	Methyl 2-furoate	$C_6H_6O_3$	125.0255	2.874	129295	81.18
5	L-2-Amino-3-methylene-hexanoic acid	$C_7H_{13}NO_2$	166.0849	4.26	11063	84.33	2-Galloylglucose	$C_{13}H_{16}O_{10}$	331.0704	3.524	11035	59.69
6	3-acetamidobutanal	$C_6H_{11}NO_2$	152.0694	4.526	95718	79.87	Thiazafluron	$C_6H_7F_3N_4OS$	299.044	4.565	16538	68.6
7	Isocarbamid	$C_8H_{15}N_3O_2$	186.122	4.578	47645	74.41	Thiofanox	$C_9H_{18}N_2O_2S$	217.1004	4.879	20810	87.29
8	Isobutyl N- methyl anthranilate	$C_{12}H_{17}NO_2$	208.1316	4.74	59111	89.11	Benzoylmalic acid	$C_{11}H_{10}O_6$	283.0488	5.033	12085	61.42
9	N-Acetylserotonin	$C_{12}H_{14}N_2O_2$	219.1122	5.055	572526	93.59	Pyraclonil	$C_{15}H_{15}ClN_6$	359.1027	5.069	66908	67.32
10	Indoleacrylic acid	$C_{11}H_9NO_2$	188.0701	5.057	551099	95.11	Unknown Comp. 5.17	$C_6H_{10}O$	143.071	5.254	7385	83.58
11	Aspergillic acid	$C_{12}H_{20}N_2O_2$	247.143	5.399	350454	91.03	Ethyl methanesulfonate	$C_3H_8O_3S$	169.0162	5.482	17599	83.61
12	Primidone	$C_{12}H_{14}N_2O_2$	219.1118	5.405	240774	94.81	3,8-Dimethyldec-7-en-1-yl trihydrogen diphosphate	$C_{12}H_26O_7P_2$	343.1074	5.528	11559	80.85
13	Erinacine P	$C_{27}H_{40}O_8$	493.2789	5.453	952200	83.95	DL-3,4-Dihydroxymandelic acid	$C_8H_8O_5$	183.032	5.641	11216	66.79
14	6-Methylquinoline	$C_{10}H_9N$	144.08	5.495	165364	83.48	UDP-2-acetamido-4-amino-2,4,6-tri-deoxyglucose	$C_{17}H_{28}N_4O_{15}P_2$	635.0972	6.057	48988	74.02
15	Indoleacrylic acid	$C_{11}H_9NO_2$	188.0695	6.103	124215	94.5	2,3-Diphenyl-3-(2-pyridinyl) acrylonitrile	$C_{20}H_{14}N_2$	327.1122	6.105	13953	88.2
16	3-Butylpyridine	$C_9H_{13}N$	158.0956	6.263	124557	73.47	N1-(5-Phospho-a-D-ribosyl)-5,6- dimethyl benzimidazole	$C_{14}H_{19}N_2O_7P$	403.09	6.428	13153	93.75
17	3-Hydroxy monoethylglycyl xylidide (3-Hydroxy-MEGX)	$C_{12}H_{18}N_2O_2$	245.1269	6.278	62459	82.15	Unknown Comp. 5.18		643.1544	6.982	86386	-

Table 5. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
18	Baptifoline	$C_{15}H_{20}N_2O_2$	261.1585	6.327	25511	80.31	Tenitramine	$C_{10}H_{20}N_6O_{12}$	475.1324	7.264	121531	57.5
19	Valyl-Tyrosine	$C_{14}H_{20}N_2O_4$	303.132	6.498	33164	82.67	Dapsone	$C_{12}H_{12}N_2O_2S$	307.1767	8.672	15875	88.58
20	Kuwanon Z	$C_{34}H_{26}O_{10}$	595.1618	6.647	128363	85.06	3-(4-Chloro-benzyl)-5-(2-methoxy-phenyl)-[1,2,4] oxadiazole	$C_{16}H_{13}ClN_2O_2$	299.0603	9.463	14385	56.34
21	Ginkgolide C	$C_{20}H_{24}O_{11}$	463.1204	6.796	125324	97.7	3-Deoxy-D-manno-octulosonate	$C_8H_{14}O_8$	283.0654	10.755	45508	74.29
22	7-Dehydrologanin tetraacetate	$C_{25}H_{32}O_{14}$	579.1669	6.798	75442	95.06	Phytolaccoside D2	$C_{42}H_{66}O_{15}$	809.4457	11.263	56997	51.47
23	Aspergillic acid	$C_{12}H_{20}N_2O_2$	247.1426	7.015	90363	95.73	Fungichromin	$C_{35}H_{58}O_{12}$	669.3864	11.505	15184	63.78
24	Byakangelicin	$C_{17}H_{18}O_7$	357.0944	7.029	46604	98.64	PIP (18:0/16:1(9Z))	$C_{43}H_{82}O_{16}P_2$	961.5099	11.591	140651	65.27
25	Calendoflaside	$C_{28}H_{32}O_{15}$	609.1796	7.104	178527	78.71	TR-Saponin B	$C_{52}H_{80}O_{20}$	1023.508	11.66	13527	61.12
26	Pallidol 3-glucoside	$C_{34}H_{32}O_{11}$	639.1877	7.325	73956	77.59	9Z-Octadecenedioic acid	$C_{18}H_{32}O4$	311.2276	11.745	69250	57.12
27	Evodiamine	$C_{19}H_{17}N_3O$	326.1272	8.031	115577	94.4	PIP (18:0/16:1(9Z))	$C_{43}H_{82}O_{16}P_2$	961.5077	11.968	19488	67.05
28	Unknown Comp. 5.2		785.4147	8.42	64721	-	Oleanolic acid 3- [rhamnosyl-(1->4)-glucosyl-(1->6)-glucoside]	$C_{48}H_{78}O_{17}$	925.5286	12.005	13773	53.75
29	3',4'-Dihydrodiol	$C_{15}H_{14}N_2O_4$	309.0854	8.507	118178	94.49	Dibutyl decanedioate	$C_{18}H_{34}O_4$	313.2429	12.397	26039	62.84
30	Unknown Comp. 5.3		618.2711	9.193	45051	-	3-O-p-trans-Coumaroylalphitolic acid	$C_{39}H_{54}O_6$	617.3916	14.778	19537	62.28
31	z2-Tocopherol	$C_{28}H_{48}O_2$	439.3543	10.442	63660	99.33	α-Linolenic Acid	$C_{18}H_{30}O_2$	277.2204	16.751	172298	72.52
32	Unknown Comp. 5.4		434.288	10.579	14063	-	Linalyl caprylate	$C_{18}H_{32}O_2$	279.2366	17.652	159314	66.78
33	Prunetin	$C_{16}H_{12}O_5$	285.0745	10.653	105884	93.53	Palmitic Acid	$C_{16}H_{32}O_2$	255.2364	18.471	262648	69.17
34	(5b,7a,12a)-2-(3-methoxyphenyl)-2-oxoethyl ester-7,12-dihydroxy-cholan-24-oic acid	$C_{33}H_{48}O_6$	541.3603	10.944	70928	56.05	Unknown Comp. 5.19		281.2552	18.616	776956	-
35	15-Oxo-21-hydroxymabiogenin 3- [rhamnosyl-(1->6)-glucoside]	$C_{42}H_{66}O15$	811.444	11.455	118335	86.7	Pipercitine	$C_{23}H_{43}NO$	394.3384	18.644	224443	56.74
36	(S)-Auraptenol	$C_{15}H_{16}O_4$	283.0952	11.794	253551	94.1	Imperialine	$C_{27}H_{43}NO_3$	428.3234	18.728	193580	57.34

Table 5. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
37	Panaxydol linoleate	$C_{35}H_{54}O_3$	545.3919	11.939	214948	68.35	Petroselinic acid	$C_{18}H_{34}O_2$	281.2536	18.932	698039	58.66
38	Unknown Comp. 5.5		518.3654	12.047	89148	-	Antibiotic X 14889D	$C_{33}H_{58}O_7$	611.4181	20.719	85888	65.04
39	Unknown Comp. 5.6		356.314	12.648	181300	-						
40	Terminaline	$C_{23}H_{41}NO_2$	364.3188	13.128	110174	86.14						
41	Unknown Comp. 5.7		358.3297	13.284	113619	-						
42	Unknown Comp. 5.8		366.3343	13.756	64780	-						
43	Oleoyl Ethanolamide	$C_{20}H_{39}NO_2$	326.3036	14.074	118512	91.18						
44	Unknown Comp. 5.9		368.3513	14.402	473651	-						
45	17-Hydroxylinolenic acid	$C_{18}H_{30}O_3$	295.2256	14.764	43260	90.82						
46	3-Ketosphinganine	$C_{18}H_{37}NO_2$	322.2726	14.843	70230	86.75						
47	Unknown Comp. 5.10		520.3365	15.095	47047	-						
48	Sphinganine	$C_{18}H_{39}NO_2$	324.2879	15.746	78521	94.44						
49	23-Acetoxysoladulcidine	$C_{29}H_{47}NO_4$	496.3366	16.249	154326	76.18						
50	Mycinamicin VII	$C_{29}H47NO_7$	522.3523	16.322	94668	50.23						
51	Stearic acid	$C_{18}H_{36}O_2$	307.2615	16.536	31115	78.73						
52	Unknown Comp. 5.11		522.3534	16.692	756772	-						
53	2R-hydroxy-stearic acid	$C_{18}H_{36}O_3$	323.2565	17.286	61595	82.85						
54	Unknown Comp. 5.12		296.2932	17.789	96513	-						
55	N, N-Dimethylsphingosine	$C_{20}H_{41}NO_2$	328.3192	17.99	41481	89.14						
56	Unknown Comp. 5.13		382.3293	18.051	79696	-						
57	Unknown Comp. 5.14		396.345	18.387	122053	-						
58	Imperialine	$C_{27}H_{43}NO_3$	430.3288	18.442	112867	83.92						
59	Unknown Comp. 5.15		458.3599	19.451	54366	-						
60	Unknown Comp. 5.16		424.3759	19.594	73177	-						

Table 6. HRLCMS QTOF Compounds list of hydroalcoholic extract of classically processed *Abrus precatorius* L. black seeds

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
1	Anthranilic acid	$C_7H_7NO_2$	138.0544	1.189	150545	85.65	Gallic acid	$C_7H_6O_5$	169.0158	2.063	99442	87.75
2	Pirbuterol	$C_{12}H_{20}N_2O_3$	241.1533	1.238	12496	91.05	Narcobarbital	$C_{11}H_{15}BrN_2O_3$	347.0248	2.423	15021	66.92
3	2-Galloylglucose	$C_{13}H_{16}O_{10}$	355.0624	1.8	15177	90.59	Ellagic acid	$C_{14}H_6O_8$	361.021	2.861	1389	79.24
4	Dukunolide C	$C_{28}H_{28}O_{11}$	541.1711	1.866	43750	90.65	UDP-2-acetamido-4-amino-2,4,6-tri-deoxyglucose	$C_{17}H_{28}N_4O_{15}P_2$	635.0968	5.848	10511	68.7
5	N-D-Glucosylarylamine	$C_{12}H_{17}NO_5$	256.117	2.156	17772	84.21	Bakers yeast extract	$C_{19}H_{14}O_2$	273.0911	5.975	788	79.85
6	Ciceritol	$C_{19}H_{34}O_{16}$	541.1712	2.194	31128	85.84	Canavalioside	$C_{26}H_{42}O_{12}$	545.2676	6.12	23851	56.38
7	Miserotoxin	$C_9H_{17}NO_8$	268.1035	2.735	17561	86.58	4-(4-Hydroxyphenyl)-2-butanone O- [2-galloyl-6-p- coumaroylglucoside]	$C_{32}H_{32}O_{13}$	623.1712	6.605	23147	64.37
8	N-Acrylylglycine methyl ester	$C_6H_9NO_3$	144.0649	2.885	10801	76.67	Aprepitant	$C_{23}H_{21}F_7N_4O_3$	593.1598	6.646	16458	72.38
9	S-4-Hydroxymephenytoin	$C_{12}H_{14}N_2O_3$	235.1077	4.289		98.45	Unknown Comp. 6.11		643.1545	6.943	104063	-
10	PAB / 4-Aminobenzoic acid	$C_7H_7NO_2$	138.0552	4.468	100118	87.21	6-beta-D- Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone	$C_{23}H_{24}O_{11}$	475.1336	7.214	243891	50.74
11	Benzocaine	$C_9H_{11}NO_2$	166.0863	4.523	175602	99.87	Isoswertisin 2"-O-rhamnoside	$C_{28}H_{32}O_{14}$	637.1877	7.233	30210	53.14
12	N-Acetylserotonin	$C_{12}H_{14}N_2O_2$	219.1134	5.116	692690	98.08	Canaliculatol	$C_{42}H_{32}O_9$	679.2002	7.705	49936	76.28
13	Indoleacrylic acid	$C_{11}H_9NO_2$	188.071	5.117	619049	98.7	alpha-L- Rhamnopyranosyl-(1->2)-beta-D-galactopyranosyl-(1->2)-beta-D-glucuronopyranoside	$C_{18}H_{30}O_{16}$	547.1547	7.86	18125	81.97
14	Aspergillic acid	$C_{12}H_{20}N_2O_2$	247.1446	5.395	295009	71.44	Tenitramine	$C_{10}H_{20}N_6O_{12}$	475.1324	7.94	16790	58.59
15	Mucronine B	$C_{28}H_{36}N_4O_4$	493.2824	5.457	1066242	92.73	5-Amino-1-ribofuranosylimidazole-4-carboxyamide	$C_9H_{14}N_4O_6$	333.1034	8.61	24811	84.49
16	6-Methylquinoline	$C_{10}H_9N$	144.0812	5.795	153365	87.07	Glucoheptonic acid	$C_7H_{14}O_8$	285.0817	8.961	33001	85.89
17	Fulvine	$C_{16}H_{23}NO_5$	310.1654	5.846	174710	98.71	Urate-3- ribonucleoside	$C_{10}H_{12}N_4O_7$	299.0615	9.394	45856	83.44
18	Azobenzene	$C_{12}H_{10}N_2$	183.0923	5.863	264971	92.69	Corchorifatty acid F	$C_{18}H_{32}O_5$	327.2232	9.48	26656	53.3
19	Samin	$C_{13}H_{14}O_5$	251.0917	5.868	66828	88.19	Sulfaphenazole	$C_{15}H_{14}N_4O_2S$	313.0767	10.466	16197	91.07

Table 6. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
20	Phenmedipham	$C_{16}H_{16}N_2O_4$	301.1188	6.04	333113	98.81	3-Deoxy-D-manno-octulosonate	$C_8H_{14}O_8$	283.0658	10.72	51320	82.13
21	7-(Methylthio)heptane-nitrile	$C_8H_{15}NS$	158.097	6.136	308911	49.73	Phytolaccoside D2	$C_{42}H_{66}O_{15}$	809.4459	11.274	29053	52.69
22	6-Methylquinoline	$C_{10}H_9N$	144.0813	6.181	350434	85.93	Oleanolic acid 3-[rhamnosyl-(1->4)-glucosyl-(1->6)-glucoside]	$C_{48}H_{78}O_{17}$	925.5332	11.557	111505	50.29
23	Cyclo(L-Phe-L-Pro)	$C_{14}H_{16}N_2O_2$	245.1289	6.277	188252	86.11	PIP (18:0/16:1(9Z))	$C_{43}H_{82}O_{16}P_2$	961.5108	11.587	243709	62.7
24	Biorobin	$C_{27}H_{30}O_{15}$	595.1665	6.655	101175	98.81	11S-HpODE	$C_{18}H_{32}O_4$	311.2283	11.809	113694	54.97
25	Scoparin 2"-glucoside	$C_{28}H_{32}O_{16}$	625.1766	6.658	46096	99.49	PIP (18:1(9Z)/16:1(9Z))	$C_{43}H_{80}O_{16}P_2$	959.4923	12.329	16056	61.49
26	6-Cinnamoyl-1-galloylglucose	$C_{22}H_{22}O_{11}$	463.1237	6.801	108677	98.56	MG (15:0/0:0/0:0)	$C_{18}H_{36}O_4$	315.2586	13.229	12633	63.77
27	Chrysoeriol 7-O-neohesperidoside	$C_{28}H_{32}O_{15}$	609.1834	7.009	832581	91.34	3,6-Epoxy-5,5',6,6'-tetrahydro-b, b-carotene-3',5,5',6'-tetrol	$C_{40}H_{58}O_5$	617.4139	13.871	20353	59.09
28	cis-Miyabenol C	$C_{42}H_{32}O_9$	681.203	7.708	271131	42.67	α-Linolenic Acid	$C_{18}H_{30}O_2$	277.2217	16.708	321808	61.44
29	Retigabine	$C_{16}H_{18}FN_3O_2$	326.1295	8.016	285319	83.85	Hexazinone	$C_{12}H_{20}N_4O_2$	311.1729	17.201	51227	91.25
30	Koryoginsenoside R1	$C_{46}H_{76}O_{15}$	868.5075	8.363	100867	52.02	Linalyl caprylate	$C_{18}H_{32}O_2$	279.2371	17.641	148878	62.41
31	Unknown Comp. 6.1		706.4534	8.396	59960	-	4-Dodecylbenzenesulfonic acid	$C_{18}H_{30}O_3S$	325.1888	18.132	56058	63.35
32	Novaluron	$C_{17}H_9ClF_8N_2O_4$	493.0171	9.245	97235	62.92	Isopalmitic acid	$C_{16}H_{32}O_2$	255.2373	18.443	319378	61.47
33	Solanidine	$C_{27}H_{43}NO$	398.3429	9.666	411336	96.26	Hydroquinidine	$C_{20}H_{26}N_2O_2$	325.1894	18.477	272803	66.03
34	Wogonin	$C_{16}H_{12}O_5$	285.0763	10.669	105079	98.61	Unknown Comp. 6.12		281.256	18.617	806469	-
35	13-beta-D-Glucosyloxydocosanoate	$C_{28}H_{54}O_8$	541.3638	11.009	76230	55.4	Unknown Comp. 6.13		394.3401	18.653	256489	-
36	Aspulvinone E	$C_{17}H_{12}O_5$	297.0761	11.729	55354	91.98	Imperialine	$C_{27}H_{43}NO_3$	428.3253	18.698	223120	51.84
37	Chrysin dimethyl ether	$C_{17}H_{14}O_4$	283.097	11.797	213248	98.89	Unknown Comp. 6.14		321.2253	18.926	13524	-
38	Panaxydol linoleate	$C_{35}H_{54}O_3$	545.395	11.961	135009	93.99	Unknown Comp. 6.15		281.2545	18.977	559658	-
39	dl-alpha-Tocopherol nicotinate	$C_{35}H_{53}NO_3$	558.3847	12.03	146087	48.13	Avocadene 2-acetate	$C_{19}H_{36}O_4$	327.2598	19.09	38437	57.67
40	Unknown Comp. 6.2		525.3683	12.251	44964	-	MG (18:2(9Z,12Z)/0:0/0:0) [rac]	$C_{21}H_{38}O_4$	353.2763	19.209	203087	55.1
41	Unknown Comp. 6.3		534.2707	13.974	379843	-	Petroselinic acid	$C_{18}H_{34}O_2$	281.2537	19.297	178335	58.35

Table 6. Continued...

S. No	Positive ion mode						Negative ion mode					
	Compound	Formula	M/z +ve	RT	Abund	Score	Compound	Formula	M/z -ve	RT	Abund	Score
42	Oleoyl Ethanolamide	$C_{20}H_{39}NO_2$	326.3059	14.053	228902	97.32	14,19-Dihydroa spidospermatine	$C_{21}H_{28}N_2O_2$	339.2057	19.627	84910	73.83
43	isepamicin	$C_{22}H_{43}N_5O_{12}$	592.2754	14.145	196413	68.05						
44	Retapamulin	$C_{30}H_{47}NO_4S$	518.3243	14.315	231587	59.27						
45	Unknown Comp. 6.4		368.3527	14.472	324752	-						
46	Unknown Comp. 6.5		520.3395	15.305	302464	-						
47	23-Acetoxysoladulcidine	$C_{29}H_{47}NO_4$	496.3399	16.111	221847	96.14						
48	Unknown Comp. 6.6		522.3556	16.114	243347	-						
49	Unknown Comp. 6.7		1043.706	16.671	461622	-						
50	Unknown Comp. 6.8		296.295	17.783	114191	-						
51	Unknown Comp. 6.9		512.5034	17.868	76794	-						
52	Unknown Comp. 6.10		458.3637	19.44	91438	-						

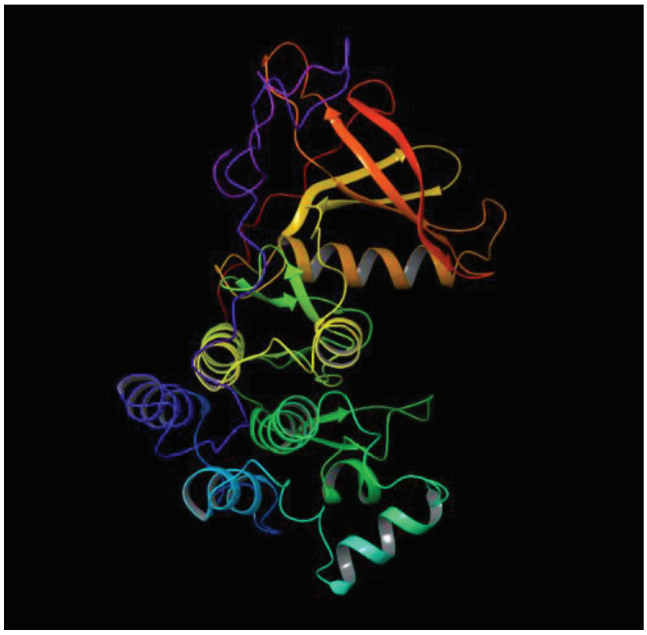


Figure 5. Endothelial growth factor receptor in the 5XDK Pdb format.

physiological changes. Hence, it has become an important need to study the interactions of various molecules with EGFR[23].

The amino acids such as Glu and Asp were found to be negatively charged and Gln, Thr, Ser, His, Asn, and Gly are polar and Leu, Met, Pro, Phe, Cys, Ala, Val are hydrophobic. It was observed that more than one hydrogen bonds are formed between the hydroxy groups of the molecules and negatively charged amino acids such as Asp, Glu and only in the cases of ellagic acid and Scoparin 2 glucoside, two hydrogen bonds are formed between Met793 and two hydroxyl groups. Hence by comparing the number of hydrogen bonds formed and the properties of the hydrogen bonds with the Glide scores of selected molecules, it is understandable that the docking scores of higher sstabilities got expressed in the molecules with more stable hydrogen bonds. The Standard ligand (8JC) which is also called Rociletinib forms two hydrogen bonds one with Asp855 and another with Lys728 which leads to the glide score of -4.3598.

Pallidol 3-glucoside is a phenolic glycoside that has a phenolic structure with a glycosyl moiety. It is an extremely weak base with water solubility of 0.11g/L with a log P value of 2.55 to 3.05[29]. It is found in alcoholic beverages normally and is a naturally occurring dimer of resveratrol. It has been reported with antioxidant and anti-fungal activities. The antioxidant activities were reported to be executed by quenching reactive oxygen species in a singlet state[30]. Whereas the dimer Resveratrol was reported to exhibit various properties such as antitumor, antiviral, antioxidant, and phytoestrogenic activities[31]. Pallidol is a glucoside molecule with a molecular mass of 616.3 g/mol, with a hydrogen bond donor count of 9 and a hydrogen bond acceptor count of 11. Pallidol has shown a glide g score value of -7.91946 as the molecule with higher affinity in the target site, which can widely act through the EGFR-related pathways. As per the HRLCMS data it was observed that the hydroalcoholic extract of black seeds has 0.499% of this metabolite. Next to that ellagic acid is found to be highly bound within the receptor site. It is a most commonly occurring polyphenol widely present in many fruits, seeds, nuts, and beverages. It has been promoted as a dietary supplement in many products. It has been reported to possess various activities such as antioxidant, liver protectant activity, anti-steatosis, anti-fibrinogenic, anti-cancer and anti-viral activities. It acts through various mechanisms such as free radical scavenging activity, regulation of phase I and II enzymes, modulation of cytokines such as proinflammatory and profibrotic and regulating various biochemical pathways[32,33]. It forms four hydrogen bonds within the target site of present interest and is present in 0.6309% of red seed, 0.1536% of processed red seed and 0.1476% of processed black seed extracts. The pharmacological data about 6'-Methoxy polygoacetophenoside is not widely available and this metabolite remains less explored. It is present in red seed extract at a concentration of 1.8934%. Chrysoeriol 7-O-neohesperidoside which is also called buddlenol C belongs to the phytochemical classification of furanoid lignans or O- O-glycosides It is a secondary metabolite that may serve as a defence or signalling molecule and is present in the red seed extract at the concentration of 9.4902%, white seed extract at 18.16356%, processed white seed extract at 9.8472% and processed black seed extract at 9.1763%. So far very few works have been published on Chrysoeriol 7-O-neohesperidoside[34,35]. This molecule is found in many cereal varieties such as corn, millet, oats, red rice, soybeans etc and herbs such as amaranth, teff and quinoa. 6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone of Flavonoids C-glycoside organic compounds is present in white seed extract at 2.25976% and processed black seed extract at 9.5025%. It is also known as 7,3'-Di-O-Methylisoorientin. It is found in other plant species such as *Eichinodorus macrophyllus* with other compounds such as swertiajaponin, swerticin,

and saponarin and this species was found to exert biological activities such as inhibition of central and peripheral mechanisms of nociception and found to be active in oedema, pain, and inflammation[36-38].

Scoparin 2"-glucoside is present in the processed black seed extract at a concentration of 0.5265%. It belongs to the class of flavonoid 8-c–glycosides that contain a carbohydrate moiety which is linked to the 2-phenylchromen-4-one flavonoid backbone. It is detected in various cereals which makes this compound an effective biomarker. It is found in various citric fruits such as sanguinello, Taroco blood orange, Mediterranian sweet lemon, Amazonian palm berry, and bergamot and is found to exert antioxidant properties[39-45]. cis-Miyabenol C belongs to a class of 2-aryl benzofuran flavonoids. It is a familiar molecule that is found in grapes, fruit of Fennel and other herbs and spices. It shows protein kinase C inhibitory activity, antiproliferative effect on cancer cells such as bladder cancer, and lung cancer and antioxidant activity[46-48]. In processed white seed extract it is present in 0.9457% and in processed black seeds in 0.5265%. PIP (18:0/16:1(9Z)) is a phosphatidyl inositol phosphate that is generated from phosphatidyl inositols. PIP (18:0/16:1(9Z)) consists of one chain of oleic acid and one chain of palmitic acid at the C1 and C2 positions. The oleic acid moiety is found to derive from various vegetable oils like olive oil and canola oil while the palmitic acid moiety widely exists in different animal fats like fish oil and mineral fats. The PIP is an important source of diacyl glycerols which act as signalling molecules via the pathways of phospholipase C enzymes[49]. It is present in various extracts such as red seed, processed red, black seed and processed black seed extracts at 1.5311%, 1.6526%, 1.7665% and 1.2063% respectively. Phlorhizin is an aryl beta D glucoside of phloretin. It is found to have various biological activities such as erythrocyte membrane stabilising activity and the lethal dose was found to be more than 500mg/kg when administered intraperitoneally in mice[50-52]. In processed red seed extracts it is present at the concentration of 0.3882%. Phloroacetophenone 6'-[xylosyl-(1->6)-glucoside] which is present at 0.878862% in white seed extract is a phenolic glycoside with a molecular weight of 490g/mol and found to be detected in different fats and oils. However, the activities of this plant metabolite are not widely explored[53].

Paeonolide is a plant glycoside that contains alpha 1 arabinopyranoside subunit found in the white seed extract at the concentration of 0.992934%. It is found to exist in plant species such as *Paeonia saffruticosa* from the ripe fruits. It acts on bone-forming cells as a regulator of the alpha 1 subunit of core binding factor. It has shown no cytotoxicity in free osteoblast[54,55]. 2-[3-Ethyl-5-(4-methoxyphenyl)-1H-pyrazol-4-yl] phenol is a pyrazol moiety that has an important role as a metabolite. It belongs to the categories of phenols, pyrazoles and monomethoxybenzenes. This molecule has been studied for its antiviral activity and growth inhibition activity of HEL cells that have undergone val617phe mutation in jak2[56]. In white seed extract, it is present in 0.554805%. Biorobin is found to exist in various plant species such as *Anthyllis henoniana, Crotalaria trichotoma, Gymnema sylvestre*, *Monteverdia ilicifolia* etc. Various extracts of *Anthyllis henoniana* were found to have various pharmacological activities such as anti-microbial activity and anti-bacterial and anti-fungal activities. Biorobin was reported to have anti-inflammatory activity in RAW 264.7 cells of mouse[57,58]. It is expressed in red seed and processed black seed extracts at the concentration of 0.7656% and 0.7281%.

Nicotiflorin is a flavonoid that is found in many plant species such as *Visnea mocanera* etc and popularly known as Kaempferol-3-o-rutinoside.it is reported for various biological activities such as acute myocardial infarction, hepatoprotective activity etc[59-61]. It was found in the white and processed white seed extracts at 4.941% and 1.7477% respectively. Biorobin and nicotiflorin have the same molecular formula but are detected only on different ionisation modes and both are found to be kaempferol derivatives. Biliverdin-IX-α belongs to the class of organic compounds namely bilirubins that contain dicarboxylic acyclic tetrapyrrole derivative. It acts on various targets such as heme oxygenase 1, myoglobin and flavin reductase (NADPH). Through interaction with biliverdin reductase, it leads to various signalling pathways of anti-inflammatory response. It is found in various spices and herbs such as angelica, garlic, lemongrass, anise saffron, oils and crops etc[62,63]. In white and processed white seed extracts it was found in 0.6969% and 0.5775% respectively. Isocarbostyril found in the processed red seed extract at the concentration of 0.4974% belongs to the phytochemical category of alkaloids. It is otherwise called 1-hydroxyisoquinoline and found to possess various biological activities such as inhibition of PARP1, inhibition of DNA repair poly (ADP ribose) polymerase 1 in murine leukaemia cells, inhibition of tissue factor VII a[64,65]. Isorhamnetin 3-O-[b- D-glucopyranosyl-(1->2)-

Table 7. Computational docking values of compounds in hydroalcoholic extract of *Abrus precatorius* L. red seeds

	Red		P. Red		White		P. White		Black		P. Black	
S. No	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore
1.	cis-Sinapic acid	-5.45641	Anthranilic acid	-5.36105	S-4-Hydroxy mephenytoin	-6.02576	S-4-Hydroxy mephenytoin	-6.02576	Anthranilic acid	-5.36105	Isocitrate	-3.89417
2.	PAB / 4-Amino benzoic acid	-5.52924	Butethal	-5.92977	N-(1-Deoxy- 1 -fructosyl) phenylalanine	-5.99547	Methyl 2-furoate	-4.82846	3-acetami dobutanal	-4.5934	Anthranilic acid	-5.36105
3.	N-(1-Deoxy-1- fructosyl) phen ylalanine	-4.67521	Isobutyl N- methyl anthranilate	-5.565	L-phe nylalanyl-L-proline	-5.47932	Hydrox yatrazine	-4.54503	Isocarbamid	-6.06217	PAB / 4-Amino benzoic acid	-5.52924
4.	1,3-Diphen ylpropane	-5.15301	Isocarbostyril	-6.85086	Methyl 2-furoate	-4.82846	N-Acetyl serotonin	-6.06123	Indoleacrylic acid	-6.33982	Benzocaine	-5.37826
5.	Indole acrylic acid	-6.33982	p-Amino benzamidine	-5.75682	N-Acetyl serotonin	-6.06123	Indoleacrylic acid	-6.33982	Aspergillic acid	-5.50157	N-Acetyl serotonin	-6.06123
6.	Euglobal-Ia1	-5.77234	Aspergillic acid	-5.50157	Indole acrylic acid	-6.33982	Maculosin	-6.2783	Primidone	-5.52583	Indole acrylic acid	-6.33982
7.	Aspergillic acid	-5.50157	Indoleacrylic acid	-6.33982	Maculosin	-6.2783	Sumatriptan	-6.67405	Erinacine P	-4.17955	Euglobal-Ia1	-5.77234
8.	Mucronine B	-4.38517	Erinacine P	-4.17955	Erinacine P	-4.17955	Erinacine P	-4.17955	6-Methyl quinoline	-6.02479	Aspergillic acid	-5.50157
9.	N-Acetyl serotonin	-6.06123	Primidone	-5.52583	Azobenzene	-4.32314	Azobenzene	-4.32314	Valyl-Tyrosine	-4.69529	Mucronine B	-4.38517
10.	6-Methyl quinoline	-6.02479	Fulvine	-5.18192	Kaempferol 4'-glucoside 7-rhamnoside	-6.07089	1,2-Bis (4-nitrophenyl) Ethane	-4.41233	Kuwanon Z	-5.80439	6-Methyl quinoline	-6.02479
11.	1-Naph thylamine	-4.82144	Samin	-6.65732	Ginkgolide C	-4.66584	Ginkgolide C	-4.66584	Byakangelicin	-5.32697	Fulvine	-5.18192
12.	7-(Meth ylthio) heptane-nitrile	-2.87269	L-phenylalanyl-L-hydr oxyproline	-5.36395	Calendoflaside	-6.76313	O-Demethyl Puromycin	-6.6267	Calendoflaside	-6.76313	Azobenzene	-4.32314
13.	(all-E)-1,7,9-Heptad ecatriene-11,13,15-triyne	0.782484	6-Methyl quinoline	-6.02479	Harman	-5.32394	Calendoflaside	-6.76313	Pallidol 3-glucoside	-7.91946	Samin	-6.65732
14.	Biorobin	-7.08346	3-Butylpyridine	-5.11126	6-beta-D-Glucopyr anosyl-4',5-dihydroxy-3',7-dimeth oxyflavone	-7.36684	6-beta-D-Glucopyranosyl 4',5-dihydroxy-3',7- dimeth oxyflavone	-5.76015	Ginkgolide C	-4.66584	Istamycin C1	-5.16253
15.	6-Cinna moyl-1-galloylglucose	-6.90296	3-Hydroxy monoethyl glycylxylidide (3-Hydroxy -MEGX)	-6.2981	Evodiamine	-5.48993	cis-Miyabenol C	-7.30262	Evodiamine	-5.48993	Phenme dipham	-4.96864
16.	Galangin 3- [galactosyl-(1->4)-	-6.90571	Kuwanon Z	-5.80439	Retigabine	-5.18571	Evodiamine	-5.48993	3',4'-Dihy drodiol	-5.37476	7-(Methy lthio)heptane-nitrile	-2.87269

Table 7. Continued...

	Red		P. Red		White		P. White		Black		P. Black	
S. No	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore
17.	Chrysoeriol 7-O-neohes peridoside	-7.40834	Reduced pyocyanine	-5.83218	2-[3-Ethyl-5-(4-methoxyphenyl)-1H-pyrazol-4-yl] phenol	-7.16583	Harman	-5.32394	Prunetin	-6.09488	Kaempferol 3-rhamnoside 7-xyloside	-7.16753
18.	Dimoracin	-5.47277	Ginkgolide C	-4.66584	Pyrohyperforin	-2.92513	Retigabine	-5.18571	(S)-Auraptenol	-4.61475	Cyclo(L-Phe-L-Pro)	-5.74818
19.	Retigabine	-5.18571	Phlorhizin	-7.19984	4,4-Difluoropregn-5-ene-3,20-dione	-4.81476	20-hydroxy-LTE4	-4.49794	Panaxydol linoleate	-2.11256	Biorobin	-7.08346
20.	Chrysin dimethyl ether	-6.05555	Calendoflaside	-6.76313	Prunetin	-6.09488	Phenethylamine glucuronide	-6.12289	4-(4-Hydroxyphenyl)-2-butanone O- [2-galloyl-6-cinnamoylglucoside]	-5.74532	Scoparin 2"-glucoside	-7.31114
21.	Panaxydol linoleate	-2.11256	Neocarzinostatin chromophore	-5.07736	Ginsenoyne A linoleate	-2.0561	Retapamulin	-3.47986	17-Hydroxylinolenic acid	-2.02697	Chrysoeriol 7-O-neohesperidoside	-7.40834
22.	Fluticasone propionate	-3.91737	Evodiamine	-5.48993	Panaxydol linoleate	-2.11256	Mycinamicin VII	-3.91347	3-Ketosphinganine	-0.35248	cis-Miyabenol C	-7.30262
23.	LysoPE(24:0/0:0)	-4.50325	(S)-Auraptenol	-4.61475	13(S)-HpODE	-3.59492	23-Acetoxy soladulcidine	-4.36685	Mycinamicin VII	-3.91347	Retigabine	-5.18571
24.	Taxa-4(20),11(12)-dien-5Î±,13Î±-diol	-5.59959	Retapamulin	-3.47986	Terminaline	-3.86543	Oleoyl Ethanolamide	-3.34952	Actinonin	-5.08016	Novaluron	-5.00393
25.	3-Ketosphinganine	-0.35248	23-Acetoxy soladulcidine	-4.36685	6-Deoxotyphasterol	-4.11003	Lyso PE (20:4(8Z, 11Z,14Z,17Z)	-5.28576	Stearic acid	-0.71749	Solanidine	-5.18632
26.	Plaunotol	-4.51338	Mycinamicin VII	-3.91347	3-Ketosphinganine	-0.90834	Northienamycin	-6.64737	Oleoyl Ethanolamide	-3.34952	Wogonin	-6.65621
27.	Oleoyl Ethan olamide	-3.34952	3-Ketosphinganine	-0.35248	Sphinganine	-2.24775	Methionyl-Valine	-3.05017	Imperialine	-5.19801	Repaglinide	-5.28808
28.	2alpha- (Hydroxymethyl)-5alpha- androstane-3beta,17beta-diol	-4.70894	Thyroxine sulfate	-6.87552	Oleoyl Ethanolamide	-3.34952	Canavalioside	-4.93033	Gallic acid	-5.92582	Chrysin dimethyl ether	-6.05555
29.	Imperialine	-5.19801	Acetylgitaloxin	-3.20806	N, N-Dimethyl sphingosine	-3.11181	Biliverdin-IX-Î±	-7.02378	Narcobarbital	-3.93546	Panaxydol linoleate	-2.11256
30.	2-Galloylglucose	-5.65712	Gallic acid	-5.92582	L-Sorbose	-5.21987	Dihydroferulic acid 4-O-glucuronide	-6.7199	Methyl 2-furoate	-4.82846	dl-alpha-Tocopherol nicotinate	-2.42223
31.	Gallic acid	-5.92582	Ellagic acid	-7.54336	L-2-Methyl tryptophan	-7.11296	(+)-2,7-Dideoxy pancratistatin	-5.68612	Tenitramine	-2.9231	Oleoyl Ethanolamide	-3.34952
32.	Narcobarbital	-3.93546	6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-	-5.76015	Northienamycin	-6.64737	Kakuol	-5.80549	Lanceotoxin A	-5.13337	23-Acetoxy soladulcidine	-4.36685
33.	Ellagic acid	-7.54336	Fungichromin	-5.5434	2,6-dihydroxy benzoic acid	-5.214	Tenitramine	-2.9231	Fungichromin	-5.5434	Narcobarbital	-3.93546
34.	Methyl 2-furoate	-4.82846	PIP (18:0/16:1(9Z))	-7.267	Resorcinol	-5.17262	Nicotiflorin	-7.08346	PIP (18:0/16:1(9Z))	-7.267	Gallic acid	-5.92582

Table 7. Continued...

	Red		P. Red		White		P. White		Black		P. Black	
S. No	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore
35.	6'-Methoxy polygoacetophenoside	-7.4506	TR-Saponin B	-6.35768	Citrusin F	-6.2077	Isorhamnetin 3-O-[b- D glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	-6.8024	TR-Saponin B	-3.77723	Ellagic acid	-7.54336
36.	DL-3,4- Dihydroxy mandelic acid	-6.6015	Î±-Linolenic Acid	0.454837	Phloroacetophenone 6'-[xylosyl-(1->6)-glucoside]	-7.1998	Chrysoeriol 7-O-neohesperidoside	-7.40834	9Z-Octadecenedioic acid	-4.79539	6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone	-7.36684
37.	PIP (18:0/16:1(9Z))	-7.267	Auriculine	-6.02279	Paeonolide	-7.1793	Copalliferol B	-6.00715	Î±-Linolenic Acid	0.454837	Isoswertisin 2"-O-rhamnoside	-6.06686
38.	9Z-Octa decenedioic acid	-4.79539	Medicagenic acid beta-maltoside	-5.66426	beta-D-Glucopyranosyl-11-hydroxy jasmonic acid	-6.43405	Phytolaccoside D2	-6.03162	Palmitic Acid	0.188098	Fungichromin	-5.5434
39	Edulisin I	-3.84726	Linalyl caprylate	-0.05307	Canavalioside	-4.93033	Hoduloside VIII	-5.55146	Pipercitine	-2.7222	Oleanolic acid 3-[rhamnosyl-(1->4)-glucosyl-(1->6) -glucoside]	-5.57548
40.	Î±-Linolenic Acid	0.454837	Isopalmitic acid	-0.85576	Biliverdin-IX-Î±	-7.02378	Sambutoxin	-4.16349	5Î±-Pregnan-20Î±-ol-3-one	-5.37149	PIP (18:0/16:1(9Z))	-7.267
41.	Linalyl caprylate	-0.05307	Pipercitine	-2.7222	Quinacridone	-6.58137	19-Methoxypomolic acid 3-arabinoside	-4.44907	Petroselinic acid	-0.42941	11S-HpODE	-3.93876
42.	Isopalmitic acid	-0.85576	Hydroquinidine	-5.70612	Austin	-2.83073	Lyso PE (18:1(11Z)/0:0)	-5.28576			Î±-Linolenic Acid	0.454837
43.	4-Dodecyl benzenesulfonic acid	-5.20012	Imperialine	-5.19801	4-Hydroxy cinnamic acid	-6.11906	Almitrine	-4.40007			Hexazinone	-4.90612
44.	Pipercitine	-2.7222	MG (18:2(9Z,12Z) /0:0/0:0) [ra]	-4.24086	m-Coumaric acid	-5.41341	Gymnodimine	-3.75212			Linalyl caprylate	-0.05307
45.			Petroselinic acid	-0.42941	Nicotiflorin	-7.08346	Pipericine	-4.99063			Isopalmitic acid	-0.85576
46.					Diferuloylputrescine	-4.44582					Hydroquinidine	-5.70612
47.					Tenitramine	-2.9231					Imperialine	-5.19801
48.					Vanillin acetate	-6.31004					Avocadene 2-acetate	-3.19994
49.					Chrysoeriol 7-O-neohesperidoside	-7.40834					MG (18:2(9Z,12Z) /0:0/0:0) [rac]	-4.24086
50.					Isoswertisin 2"-O-rhamnoside	-6.06686					2alpha,3alpha-(Difluoromethylene)-5alpha- androstane-17beta-ol acetate	-4.24748
51.					S-Furanopetasitin	-4.06791					Petroselinic acid	-0.42941
52.					Phytolaccoside E	-5.81841						
53.					Tragopogonsaponin K	-4.42689						

Table 7. Continued...

	Red		P. Red		White		P. White		Black		P. Black	
S. No	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore	Compound	glide_ gscore
54.					Fistuloside C	-5.27671						
55.					Corchorifatty acid F	-5.81279						
56.					9,10-Dihydroxy-12,13-epoxyoctadecanoate	-4.42828						
57.					Phytolaccoside D2	-5.30839						
58.					Hoduloside VIII	-5.55146						
59.					19-Methoxy pomolic acid 3-arabinoside	-4.02375						
60.					Tingenone	-4.30218						
61.					Macamide B	-3.585						
62.					3-keto stearic acid	-0.74148						
63.					N-Hexadecanoy lpyrrolidine	-2.59453						
64.					Pipericine	-2.09879						
65.					N-(14-Methyl hexadecanoyl) pyrrolidine	-2.2582						
66.					Pipercitine	-2.09879						
67.					Imperialine	-5.19801						
68.												
69.												

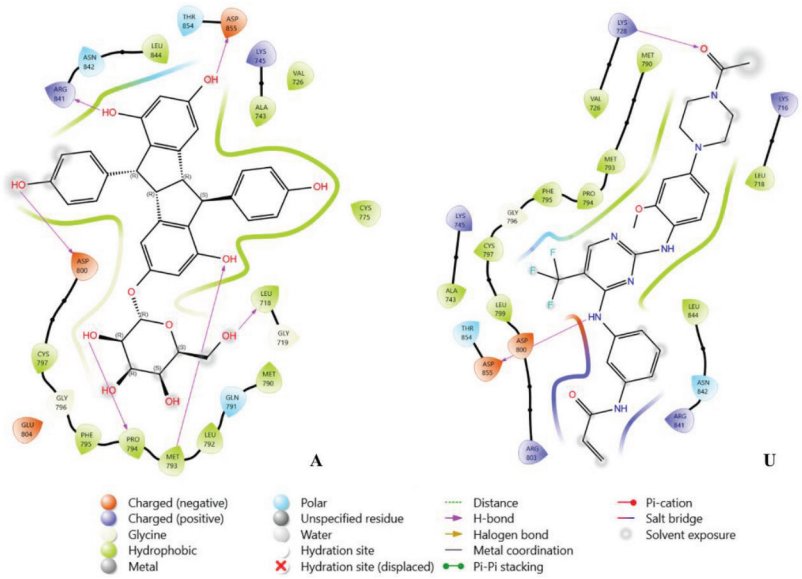


Figure 6. Ligand interaction diagrams of Pallidol 3-glucoside and Standard ligand 8JC within the grid area of EGFR.

Table 8. Ligand and protein interaction patterns of molecules present in unprocessed and processed *Abrus precatorius* L. seed extracts

	Ligand	Glide g score	Extract	QTOF Ion mode	Amino acid interaction
A	**Pallidol 3-glucoside**	-7.91946	Black	+ve	718 LEU, 719 GLY, 726 VAL, 743 ALA, 745 LYS, 775 CYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 797 CYS, 800 ASP, 804 GLU, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
B	**Ellagic acid**	-7.54336	Red, P.Red, P.Black seed	-ve	718 LEU, 726 VAL, 743 ALA, 745 LYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 796 GLY, 797 CYS, 844 LEU, 854 THR, 855 ASP
C	**6'-Methoxy polygoacetophenoside**	-7.4506	Red seed	-ve	718 LEU, 726 VAL, 743 ALA, 745 LYS, 775 CYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 796 GLY, 797 CYS, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
D	**Chrysoeriol 7-O-neohesperidoside**	-7.40834	Red, P.Black seed	+ve	718 LEU, 726 VAL, 743 ALA, 745 LYS, 775 CYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 795PHE, 796 GLY, 797 CYS, 800ASP, 801TYR, 804GLU, 85HIS, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
			White, P.white,	-ve	
E	**6-beta-D-Glucopyranosyl-4',5-dihydroxy-3',7-dimethoxyflavone**	-7.36684	White	+ve	718 LEU, 726 VAL, 728 LYS, 743 ALA, 745 LYS, 762 GLU, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 797 CYS, 800 ASP, 804 GLU, 805 HIS, 844 LEU, 854 THR, 855 ASP
			P.Black	-ve	
F	**Scoparin 2"-glucoside**	-7.31114	P.Black	+ve	718 LEU, 719 GLY, 720 SER, 721 GLY, 723 PHE, 724 GLY, 725 THR, 726 VAL, 743 ALA, 745 LYS, 791 GLN, 792 LEU, 793 MET, 794 PRO, 796 GLY, 797 CYS, 800 ASP, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP

Table 8. Continued...

	Ligand	Glide g score	Extract	QTOF Ion mode	Amino acid interaction
G	**cis-Miyabenol C**	-7.30262	P.White, P.Black	+ve	718 LEU, 719 GLY, 720 SER, 721 GLY, 723 PHE, 724 GLY, 725 THR, 726 VAL, 743 ALA, 745 LYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 796 GLY, 797 CYS, 800 ASP, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
H	**PIP (18:0/16:1(9Z))**	-7.267	Red, P.Red, Black P.Black seed	-ve	716 LYS, 718 LEU, 719 GLY, 720 SER, 721 GLY, 723 PHE, 724 GLY, 725 THR, 726 VAL, 728 LYS, 743 ALA, 745 LYS, 790 MET, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 797 CYS, 799 LEU, 800 ASP, 801 TYR, 803 ARG, 804 GLU, 805 HIS, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
I	**Phlorhizin**	-7.19984	P.Red	+ve	718 LEU, 719 GLY, 726 VAL, 728 LYS, 743 ALA, 745 LYS, 762 GLU, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 797 CYS, 844 LEU, 854 THR, 855 ASP
J	**Phloroacetophenone 6'-[xylosyl-(1->6)-glucoside]**	-7.1998	White	-ve	718 LEU, 726 VAL, 728 LYS, 743 ALA, 745 LYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 796 GLY, 797 CYS, 800 ASP, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
K	**Paeonolide**	-7.1793	White	-ve	718 LEU, 726 VAL, 743 ALA, 745 LYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 796 GLY, 797 CYS, 800 ASP, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
L	**2-[3-Ethyl-5-(4-methoxyphenyl)-1H-pyrazol-4-yl] phenol**	-7.16583	White	+ve	718 LEU, 726 VAL, 743 ALA, 745 LYS, 775CYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 797 CYS, 844 LEU, 854 THR, 855 ASP
M	**Biorobin**	-7.08346	Red seed P.Black	+ve	718 LEU, 719 GLY, 720 SER, 723 PHE, 724 GLY, 725 THR, 726 VAL, 743 ALA, 745 LYS, 762 GLU, 790 MET, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 844 LEU, 854 THR, 855 ASP, 857 GLY
N	**Nicotiflorin**	-7.08346	White P.White	-ve	718 LEU, 719 GLY, 720 SER, 723 PHE, 724 GLY, 725 THR, 726 VAL, 743 ALA, 745 LYS, 762 GLU, 790 MET, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 844 LEU, 854 THR, 855 ASP, 857 GLY
O	**Biliverdin-IX-α**	-7.02378	White P.White	-ve	718 LEU, 719 GLY, 720 SER, 723 PHE, 726 VAL, 728 LYS, 743 ALA, 745 LYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 796 GLY, 800 ASP, 844 LEU, 854 THR, 855 ASP
P	**Thyroxine sulfate**	-6.87552	P.Red	+ve	718 LEU, 719 GLY, 726 VAL, 743 ALA, 745 LYS, 762 GLU, 790 MET, 792 LEU, 793 MET, 796 GLY, 797 CYS, 800 ASP, 844 LEU, 854 THR, 855 ASP
Q	**Isocarbostyril**	-6.85086	P.Red	+ve	718 LEU, 726 VAL, 743 ALA, 790 MET, 791 GLN, 792 LEU, 793 MET, 844 LEU, 854 THR

Table 8. Continued...

	Ligand	Glide g score	Extract	QTOF Ion mode	Amino acid interaction
R	**Isorhamnetin 3-O-[b- D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]**	-6.8024	P.White	-ve	718 LEU, 719 GLY, 723 PHE, 726 VAL, 743 ALA, 745 LYS, 775 CYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 797 CYS, 800 ASP, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
S	**Calendoflaside**	-6.76313	White Black P.Red P. White	+ve	718 LEU, 719 GLY, 726 VAL, 728 LYS, 743 ALA, 745 LYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 797 CYS, 800 ASP, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP
T	**Indoleacrylic acid**	-6.33982	Red P. Red P.Whit Black P.Black	+ve	718 LEU, 726 VAL, 743 ALA, 745 LYS, 762 GLU, 766 MET, 775 CYS, 790 MET, 791 GLN, 792 LEU, 793 MET, 844 LEU, 854 THR, 855 ASP, 856 PHE
U	**Prunetin**	-6.09488	P. Red White Black	+ve	718 LEU, 726 VAL, 728 LYS, 743 ALA, 745 LYS, 762 GLU, 790 MET, 791 GLN, 792 LEU, 793 MET, 794 PRO, 795 PHE, 796 GLY, 844 LEU, 854 THR, 855 ASP
V	**Standard ligand (8JC)**	-4.35987			716 LYS, 718 LEU, 726 VAL, 728 LYS, 743 ALA, 745 LYS, 790 MET, 793 MET, 794 PRO, 795 PHE, 796 GLY, 797 CYS, 799 LEU, 800 ASP, 803 ARG, 841 ARG, 842 ASN, 844 LEU, 854 THR, 855 ASP

a-L-rhamnopyranoside] is an organic compound that belongs to the category of Flavonoid-3-o-glycosides. It is a glycoside and a member of flavonoids. It is reported to be found in *Gingko biloba*. It is detected in various fats and oils. It was reported to have free radical scavenging activity[66]. In processed white seed extract it is present in the quantity of 0.1013%.

Calendoflaside belongs to the organic compound category of flavonoid-3-0-glycoside. It was reported to be present in *Calendula officinalis* and the plant species was studied for its anti-COVID activities[67,68]. It was found in various extracts such as white, processed white, processed red and black seed extracts at the percentages of 5.9299, 3.4991, 10.0189 and 11.9973 respectively. Indoleacrylic acid is one of the best-known plant growth hormones and belongs to the category of alpha, beta-unsaturated monocarboxylic acid, and indoles. It is found in red algae, *Chondria atropurpurea* and other plant products such as canola straw. Indole acrylic acid produced *by Parabacteriodes distasonis* alleviates type II diabetes by the mechanism of activating AhR to repair intestinal barrier[69-71]. In other studies, it was reported to reduce inflammation. In the present study, it was detected in various extracts such as red, processed red, black, processed black and processed white at 11.5826, 3.3409, 6.811, 3.7819 and 12.621 percentages respectively. Prunetin was found in the processed red, white, and black seed extracts at concentrations of 0.4459, 0.5462 and 1.0633 % respectively. It belongs to the category of hydroxy isoflavone and is reported to have various activities such as an anti-inflammatory agent, and human recombinant ALDH2 inhibitor and shows various agonist characteristics at glucocorticoid receptor, and androgen receptor and acts as anti-cancer agents[72].

The herbal medicines, particularly the extracts can act like combinational therapies with many molecules. These extracts can be a very good source of molecules with notable activity against many disorders. With such a concept if the above-selected molecules of higher receptor affinity using docking studies are considered together, the total percentage areas of these molecules in red seed, processed red seed, white seed, processed white seed, black seed and processed black seed extracts are found to be 25.8938, 16.4975, 34.9637, 29.3396, 20.8024 and 25.3096 respectively as per the HR-LCMS reports.

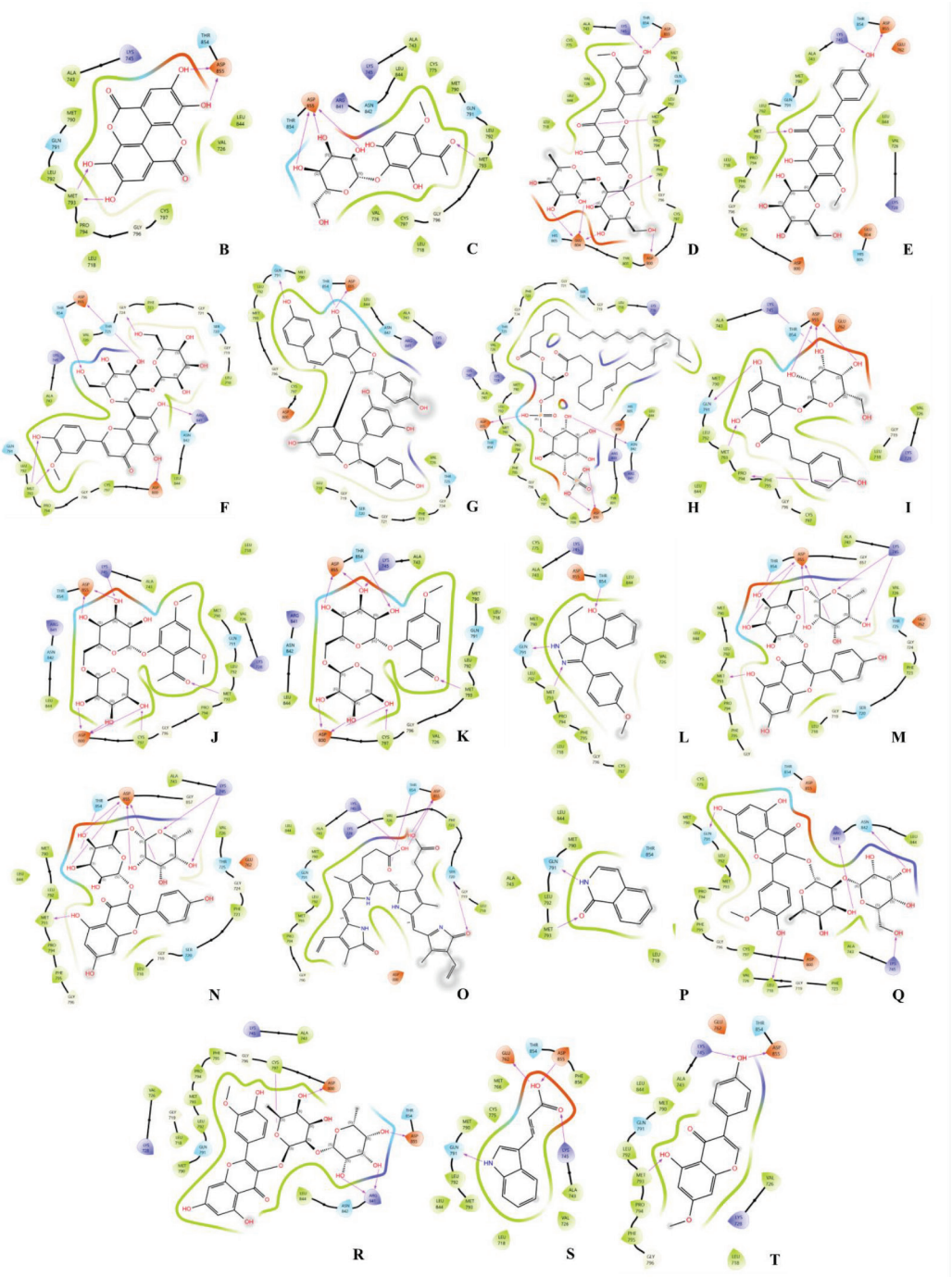


Figure 7. Structures of various metabolites represented in Table 8 in the form of target interaction diagrams within the grid area of EGFR.

5. Conclusion

It is concluded that the extracts of red, white, and black varieties of *Abrus precatorius* L. seeds that are subjected to the *Shodhana* procedure have shown large variations in phytochemical levels in comparison with unprocessed seeds and these extracts may act as a potent principle in managing cancer by acting on Epidermal Growth Factor Receptor. Among all six extracts, the white seed extract was found to possess a higher percentage of effective EGFR binding molecules followed by the processed white seed extract. Hence these extracts can be considered

effective in managing cancer by interacting with EGFR. However, further *in-vitro* and *in-vivo* evaluations can be carried out to ensure the biological activities of these extracts.

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