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Research Article

An *In silico* approach to investigating the anti-breast cancer activity of the plant genus *Spatholobus*

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Abstract

Simulating the potential anticancer action of medicines from the genus *Spatholobus* is the aim of the current investigation. The 33 bioactive compounds that make up the genus *Spatholobus* were put together from earlier research. They were analyzed to assess the probability of biological activity using the PASS server. The network analysis and ligand-protein interaction were looked at using the STITCH web server. The features of the pharmacology are evaluated using the SwissADME web server. According to these results, the substances that best meet the requirements for oral intake include medicarpin, maackiain, lupinalbin A, medioresinol, 8-omethylretusin, biochanin A, isoliquiritigenin, coumestrol, and trigraecum. The activation of caspase-3 and Bcl-2 in the apoptosis and p53 signalling pathways by the nine chemicals suggests that they have the ability to combat breast cancer.

Keywords: *Spatholobus*, bioactive compounds, network analysis, caspase-3, Bcl-2, p53

Introduction

Breast cancer has been the most prevalent ailment in 2020. 2.26 million cases and 685,000 fatalities were reported by WHO (Brentnall et al., 2013). The majority of chemotherapeutic agents used in clinical oncology kill cancer cells by activating the normal apoptosis signaling system (Chen et al., 2019; Suryanarayana et al., 2021). Popular proteins have a significant roles to play in apoptosis. The proteins include heat shock proteins, amyloid-B peptide, the Bcl family of proteins, the caspases, and the p53 gene (Christina et al., 2021). A large number of genes are automatically activated, expressed, as well as regulated during the spontaneous regulation of cell proliferation. This procedure causes organisms to undergo cellular senescence (Kim et al., 2021; Govindarasu et al., 2021). Cancerous cells might live much longer thus promote the buildup of oncogenic variants associated with defective apoptosis. Apoptosis defects could be repaired by natural ingredients, according to significant experimental findings (Cragg et al., 2006). A significant portion of the pharmacological medicines used in

cancer therapy comprises natural compounds (Sarkar, 2021). The plant belonging to the genus *Spatholobus* being one of those with potential anticancer properties (Cui et al., 2009). The chemicals from this species have been noted in certain articles to exhibit anticancer properties (Cragg et al., 2006; Daina et al., 2017). According to reports, the *Spatholobus* genus contains thirty-four species worldwide, while another five are now undergoing verification. According to earlier sources, this genus had 33 known compounds (Table 2). There are presently few articles describing the bioactivity of chemicals from plants in the *Spatholobus* genus that are anti-breast cancer. There is an acute need for the initial potential performance investigation of chemicals from the genus *Spatholobus*. Both computational and experimental methods are applicable. The goal of the current preliminary report seems to be to simulate the probable biological functions of chemicals from the genus *Spatholobus* related to breast carcinoma.

Materials and methods

Assessment of biological function using PASS server

From pubchem, all compound canonical smiles of the *Spatholobus* genus were obtained. Caspase 3 stimulant, antineoplastic, apoptosis agonist, TP53 expression enhancer, caspase 8 stimulant, and anti-carcinogenic seem to be at least some of the pharmacological activities related to apoptosis (Emami et al., 2014; Oubella et al., 2021; Thapa et al., 2021). The standard smiles were added to pass. The P_a (active) and P_i (inactive) values would appear together with the physiological and biochemical list. The P_a values in this technique were set at $P_a > 0.75$ (Yoon et al., 2004; Kore et al., 2021; Lagunin et al., 2018; Mutazahet et al., 2020). The score indicates the likelihood that a chemical would be active. The greater P_a , ever more likely bioactivity seems to be to occur. The substances exhibiting apoptosis-related activity ($P_a > 0.75$) have been chosen being used in the next steps.

Examination of the ligand-protein interaction and network

The STITCH analysis (<http://stitch.embl.de/>) was used to determine the relationships between the substances with the strongest biological activity and proteins. Cytoscape is being used to accomplish the interactions.

Assessment of pharmacological parameters

Swiss ADME web service (<http://www.swissadme.ch/>) has been used to investigate the pharmacology of active component characteristics. It contains the canonical grins of the most potent chemical. The information would have been displayed on the server and then interpreted in accordance with the best standards for acceptable oral dosing (Oubella et al., 2021) (Table 1).

Table 1. The optimum criteria of parameters for oral safe consumption as per lipinski rule

Sl No	Properties	Range
1	Molecular weight	150-500 g/mol
2	Polarity	TPSA 20-130Å ²
3	Solubilty	Log S > -6
4	Flexibility	Rotatable bonds <9
5	Lipophilicity	-0.7<XLOGP3<+5.0

Results and discussion

Table 2 lists the canonical smiles of species from the genus *Spatholobus*. There have been four species in the genus *Spatholobus* (*S. suberectus*, *S. parviflorus*, *S. sinensis*, and *S. dunn*). Maackiain, medicarpin, trigraecum, sativan,

pseudobaptigenin, genistin, naringenin, protocatechuic acid ethyl ester, coumestrol, isoliquiritigenin, lupinalbin A, and leonurisode A seem to be the chemicals of *S. suberectus* (Papaliagkas et al., 2018; Pistrutto et al., 2016; Sichaem et al., 2018). Medicarpin, 8-o-methylretusin, biochanin A, trans-4-hydroxymellein, cis-4-hydroxymellein, and coumestrol seem to be the main components of *S. parviflorus* (Tang et al., 2012). Prestegane B, (+)-medioresinol, benzeneethanol, naringenin, blumenol A, protocatechuic acid ethyl ester, liquiritigenin, protocatechuic acid, and glycyroside are among the components of *S. sinensis* (Tay et al., 2019; Yin et al., 2008). Calycosin, pyromucic acid, 1,3,5-benzenetriol, succinic acid, beta-sitosterol, and suberectin are indeed the main components of *S. suberectus* Dunn. On Table 3, the P_a value for apoptosis is displayed. There seem to be conceivably eleven substances that are caspase 3 stimulants with a P_a value greater than 0.75. In addition to suberectin, they also contain maackiain, medicarpin, trigraecum, genistin, medioresinol, glycyroside, beta-sitosterol, stigmaterol, isoliquiritigenin, and leonurisode A. Maackiain, medicarpin, genistin, medioresinol, glycyroside, trans & cis -4-hydroxymellein, isoliquiritigenin, lupinalbin A, and leonurisode A are among the anticipated compounds having P_a values of antineoplastic > 0.75. Maackiain, medicarpin, trigraecum, genistin, glycyroside, coumestrol, isoliquiritigenin, and leonurisode A are among the substances with such an anticipated P_a score of an apoptotic agonist higher than 0.75. Medicarpin, trigraecum, genistin, medioresinol, naringenin, liquiritigenin, formononetin, daidzein, calycosin, 1,3,5-benzenetriol, biochanin A, trans & cis -4-hydroxymellein, coumestrol, lupinalbin A, leonurisode A, and suberectin were amongst the expected chemicals with P_a . Particularly glycyroside and leonurisode A are indeed thought to be caspase 8 stimulants having estimated P_a values greater than 0.75. Finally, genistin, glycyroside, and leonurisode A were amongst the anticipated molecules having P_a values higher than 0.75. Medicarpin, glycyroside, maackiain, stigmaterol, lupinalbin A, leonurisode A, medioresinol, 8-O-methylretusin, biochanin A, isoliquiritigenin, coumestrol, genistin, trigraecum, and genistin seem to be the four compounds with the greatest P_a value (Table 4).

Protein interactions with pathway analysis

The proteins implicated in the apoptosis pathway are caspase-3, Bcl-2, FADD, caspase-8, TP53, and ATM (false discovery rate: 1.3×10^{-7}). Contrarily, the proteins involved in the p53 signalling pathway include caspase-3, caspase-8, TP53, MDM2, ATM, CDKN1A, and CDKN2A (false discovery rate 9.31×10^{-10}). Biochanin A and isoliquiritigenin likely induce significant Caspase 3 on both routes, with activation rates of 90.7 percent and 70.0 percent, respectively (Figure 1 & Figure 2).

Table 2. Compounds name, PubChem ID and SMILES of compounds from *Spatholobus* genus plants studied

No	Compound	pubchem CID	SMILES
1	Maackiain	91510	<chem>C1C2C(C3=C(O1)C=C(C=C3)O)OC4=CC5=C(C=C24)OC(O)C</chem>
2	Medicarpin	336327	<chem>COC1=CC2=C(C=C1)C3COC4=C(C3O2)C=CC(=C4)O</chem>
3	Trigraecum	14376438	<chem>COC1=C(C=C2C(=C1)C(=O)C=C(O2)C3=CC=CC=C3)O</chem>
4	Sativan	596401	<chem>COC1=CC(=C(C=C1)C2CC3=C(C=C(C=C3)O)OC2)OC</chem>
5	Pseudobaptigenin	5281805	<chem>C1OC2=C(O1)C=C(C=C2)C3=COC4=C(C3=O)C=CC(=C4)O</chem>
6	Genistin	5281377	<chem>C1=CC(=CC=C1C2=COC3=CC(=CC(=C3C2=O)O)OC4C(C(C(C(O4)CO)O)O)O</chem>
7	prestegane B	146425	<chem>COC1=C(C=C(C=C1)CC2COC(=O)C2CC3=CC(=C(C=C3)OC)O)O</chem>
8	(+)-medioresinol	181681	<chem>COC1=CC(=CC(=C1O)OC)C2C3COC(C3CO2)C4=CC(=C(C=C4)O)OC</chem>
9	Benzeneethanol	6054	<chem>C1=CC=C(C=C1)CCO</chem>
10	Naringenin	932	<chem>C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC=C(C=C3)O</chem>
11	Blumenol A	5280462	<chem>CC1=CC(=O)CC(C1(C=CC(C)O)O)(C)C</chem>
12	Protocatechuic acid ethyl ester	77547	<chem>CCOC(=O)C1=CC(=C(C=C1)O)O</chem>
13	Liquiritigenin	114829	<chem>C1C(OC2=C(C1=O)C=CC(=C2)O)C3=CC=C(C=C3)O</chem>
14	protocatechuic acid	72	<chem>C1=CC(=C(C=C1C(=O)O)O)O</chem>
15	Glycyroside	101939210	<chem>COC1=CC=C(C=C1)C2=COC3=C(C2=O)C=CC(=C3)OC4C(C(C(C(O4)CO)O)O)OC5C(C(CO5)(CO)O)O</chem>
16	Formononetin	5280378	<chem>COC1=CC=C(C=C1)C2=COC3=C(C2=O)C=CC(=C3)O</chem>
17	Daidzein	5281708	<chem>C1=CC(=CC=C1C2=COC3=C(C2=O)C=CC(=C3)O)O</chem>
18	Calycosin	5280448	<chem>COC1=C(C=C(C=C1)C2=COC3=C(C2=O)C=CC(=C3)O)O</chem>
19	Pyromucic acid	6919	<chem>C1=COC(=C1)C(=O)O</chem>
20	1,3,5-benzenetriol	359	<chem>C1=C(C=C(C=C1O)O)O</chem>
21	succinic acid	1110	<chem>C(CC(=O)O)C(=O)O</chem>
22	Beta-sitosterol	222284	<chem>CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C(C)C</chem>
23	Stigmasterol	5280794	<chem>CCC(C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C(C)C</chem>
24	(6aR,11aR)-medicarpin	336327	<chem>COC1=CC2=C(C=C1)C3COC4=C(C3O2)C=CC(=C4)O</chem>
25	8-O-methylretusin	5319771	<chem>COC1=CC=C(C=C1)C2=COC3=C(C2=O)C=CC(=C3OC)O</chem>
26	Biochanin A	5280373	<chem>COC1=CC=C(C=C1)C2=COC3=CC(=CC(=C3C2=O)O)O</chem>
27	Trans-4-Hydroxymellein	10262028	<chem>CC1C(C2=C(C(=CC=C2)O)C(=O)O1)O</chem>
28	Cis-4-Hydroxymellein	10420140	<chem>CC1C(C2=C(C(=CC=C2)O)C(=O)O1)O</chem>
29	Coumestrol	5281707	<chem>C1=CC2=C(C=C1O)OC3=C2C(=O)OC4=C3C=CC(=C4)O</chem>
30	Isoliquiritigenin	638278	<chem>C1=CC(=CC=C1C=CC(=O)C2=C(C=C(C=C2)O)O)O</chem>
31	lupinalbin A	5324349	<chem>C1=CC2=C(C=C1O)OC3=C2C(=O)C4=C(C=C(C=C4O3)O)O</chem>
32	Leonuriside A	14237625	<chem>COC1=CC(=CC(=C1OC2C(C(C(C(O2)CO)O)O)O)OC)O</chem>
33	Suberectin	5321538	<chem>COC1=C(O)C=C2OC(CC(=O)C2=C1)C1=CC(O)=C(O)C=C1</chem>

By proteolytically inactivating DFF45/ICAD (Fig. 3), caspase 3 starts the apoptosis process and serves as a crucial indicator of the cell's entry point into the apoptosis signalling pathway. SREBPs, caspase 6, caspase 7, and caspase 9 are just a few of the effectors that caspase-3 has been shown to cleave and activate (Yanagihara et al., 1993). Additionally, as per the apoptosis pathway, isoliquiritinigen facilitates faster (70.0 percent) with Bcl2, however the nature of the contact is unknown. The other ligands, however, don't interact with the proteins in either pathway. We suspect that STITCH's database has not yet been updated or that the most recent report is not available.

Table 5 displays the list of pharmacological characteristics of active substances. The following substances do not match the ideal conditions for pharmacological properties: glycyroside (MW>500 g, TPSA>130 Å²), stigmasterol (Log S -6, Log P3>5), leonuriside A (TPSA>130 Å²), and genistin (TPSA>130 Å²). The others, on the other hand, meet the necessary standards. Although benign prostatic hyperplasia (BPH), infection, and/or chronic inflammation can also be the reason of an increased TPSA level, it can also indicate the existence of cancer.

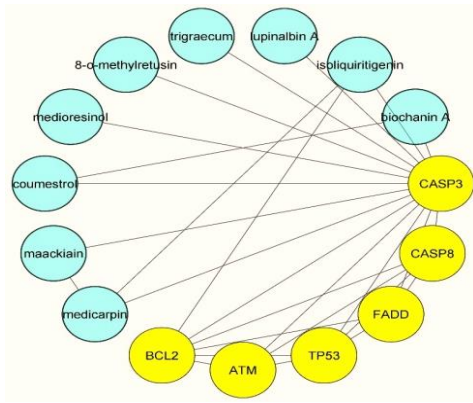


Fig. 1 Protein interactions with pathway analysis for apoptosis

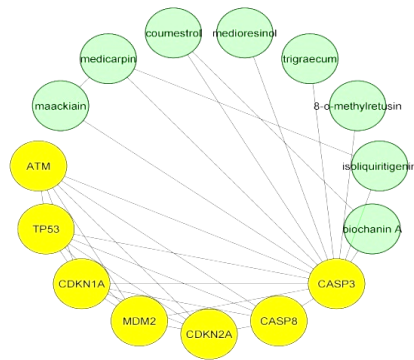


Fig. 2 Protein interactions with pathway analysis for p53

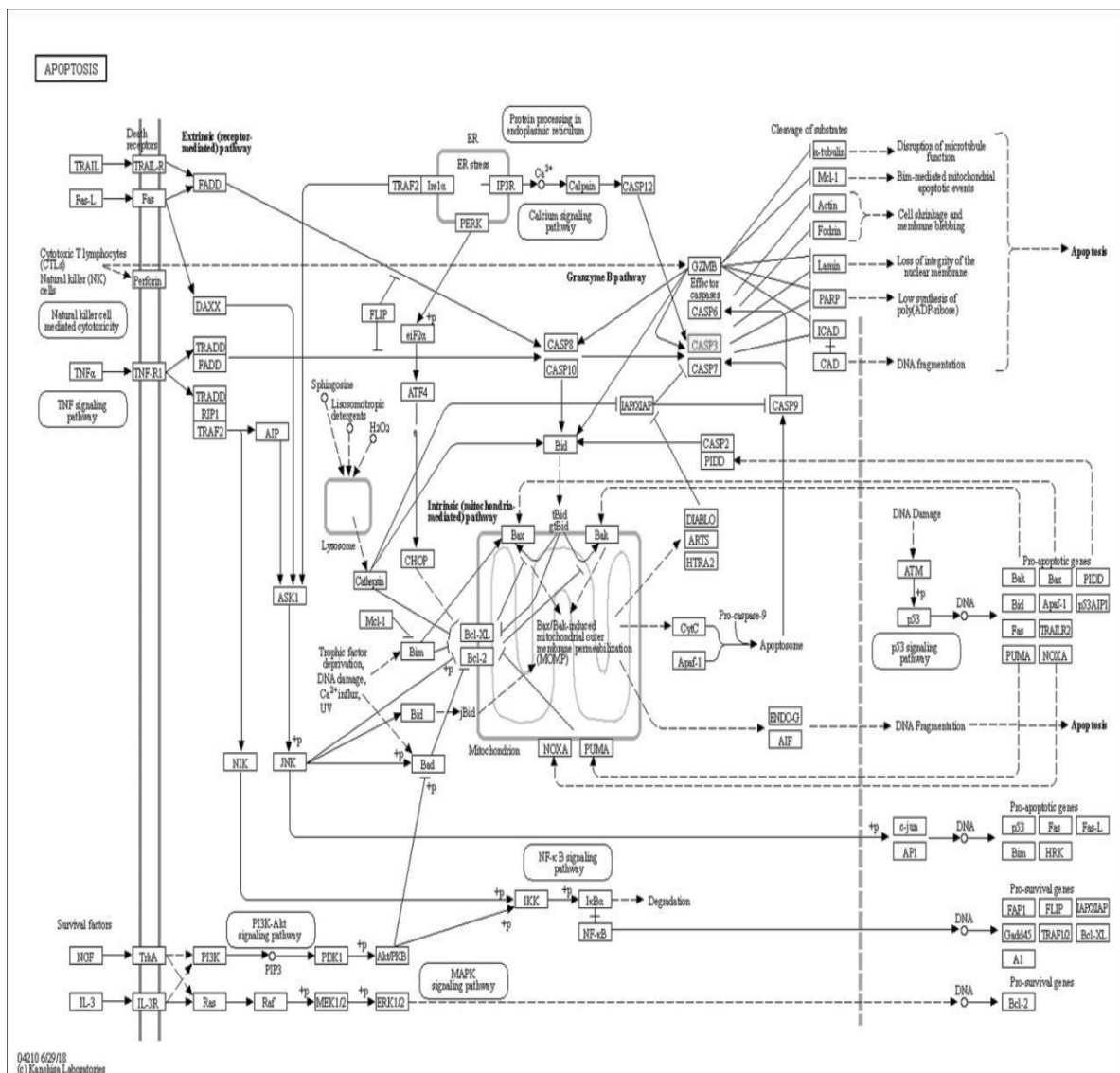


Fig. 3 Apoptosis pathway of Caspase 3

Table 3. Apoptosis-related activity screening results of all selected compounds

No	Compounds	$P_a > 0.75$					
		Caspase-3 stimulant	Antineoplastic	Apoptosis agonist	TP53 expression enhancer	Caspase-8 stimulant	anticarcinogenic
1	Maackiain	0.934	0.788	0.751	-	-	-
2	Medicarpin	0.991	0.769	0.778	0.774	-	-
3	Trigraecum	0.751	-	0.769	0.863	-	-
4	Sativan	-	-	-	-	-	-
5	Pseudobaptigenin	-	-	-	-	-	-
6	Genistin	0.763	0.814	0.757	0.912	-	0.951
7	prestegane B	-	-	-	-	-	-
8	(+)-medioresinol	0.757	0.812	-	0.800	-	-
9	Benzeneethanol	-	-	-	-	-	-
10	4,7,2'-trihydroxy-4'-methoxyisoflavone	-	-	-	-	-	-
11	Naringenin	-	-	-	0.822	-	-
12	Blumenol A	-	-	-	-	-	-
13	Protocatechuic acid ethyl ester	-	-	-	-	-	-
14	Liquiritigenin	-	-	-	0.769	-	-
15	protocatechuic acid	-	-	-	-	-	-
16	Glycyroside	0.975	0.864	0.790	-	0.857	0.922
17	Formononetin	-	-	-	0.770	-	-
18	Daidzein	-	-	0.755	0.771	-	-
19	Calycosin	-	-	0.779	0.797	-	-
20	Pyromucic acid	-	-	-	-	-	-
21	1,3,5-benzenetriol	-	-	-	0.752	-	-
22	succinic acid	-	-	-	-	-	-
23	Beta-sitosterol	0.806	-	-	-	-	-
24	Stigmasterol	0.863	-	0.753	-	-	-
25	8-O-methylretusin	-	-	0.827	-	-	-
26	Biochanin A	-	-	0.823	0.823	-	-
27	Trans-4-Hydroxymellein	-	0.790	-	0.796	-	-
28	Cis-4-Hydroxymellein	-	0.790	-	0.796	-	-
29	Coumestrol	-	-	0.811	0.769	-	-
30	Isoliquiritigenin	0.793	0.752	0.812	-	-	-
31	lupinalbin A	-	0.953	-	0.789	-	-
32	Leonuriside A	0.862	0.829	0.712	0.835	0.762	0.833
33	Suberectin	0.751	-	-	0.780	-	-

Table 4. The four highest P_a Value (>0.75) related to apoptosis

Biological Activity	The four highest P_a Value
Caspase 3 stimulant	Medicarpin (0.991), Glycyroside (0.975), Maackiain (0.934), Stigmasterol (0.863)
Antineoplastic	Lupinalbin A (0.953), Glycyroside (0.864), Leonuriside A (0.829), Medioresinol (0.812)
Apoptosis agonist	8-O-methylretusin (0.827), Biochanin A (0.823), Isoliquiritigenin (0.812), Coumestrol (0.811)
TP53 expression enhancer	Genistin (0.911), Trigraecum (0.863), Leonuriside A (0.835), Biochanin A (0.823)
Caspase 8 stimulant	Glycyroside (0.857), Leonuriside A (0.762)
Anticarcinogenic	Genistin (0.951), Glycyroside (0.922), Leonuriside A (0.833)

Table 5. Pharmacological properties of investigated bioactive compounds

No	Compound	Molecular weight (g/mol)	LogP values	Solubility (Log S)	Flexibility			Lipophilicity (Log P)
					H-bond acceptors	H-bond donors	Rotatable bonds	
1	Medicarpin	270.28	47.92 Å ²	-3.64	4	1	1	2.77
2	Glycyroside	562.52	197.74 Å ²	-2.95	13	6	8	-0.23
3	Maackiain	284.26	57.15 Å ²	-3.67	5	1	0	2.61
4	Stigmasterol	412.69	20.23 Å ²	-7.46	1	1	5	8.56
5	lupinalbin A	284.22	104.04 Å ²	-4.2	6	3	0	3.18
6	leonuriside A	332.3	138.07 Å ²	-1.2	9	5	5	-0.90
7	medioresinol	388.41	86.61 Å ²	-3.65	7	2	5	2.25
8	8-O-methylretusin	298.29	68.90 Å ²	-3.77	5	1	3	2.77
9	biochanin A	284.26	79.90 Å ²	-3.92	5	2	2	2.99
10	Isoliquiritigenin	256.25	77.76 Å ²	-3.7	4	3	3	3.18
11	Coumestrol	268.22	83.81 Å ²	-3.87	5	2	0	2.76
12	Genistin	432.38	170.05 Å ²	-3.18	10	6	4	0.86
13	Trigraecum	268.26	59.67 Å ²	-4.22	4	1	2	3.59

Conclusion

Caspase-3 and Bcl-2 are likely to be target proteins in the apoptosis and p53 signalling pathways, according to the findings of the investigation of numerous processes. This hypothesis has to be investigated in molecular docking and verified by molecular dynamic. The proviso that bioactive chemicals from plants of the genus *Spatholobus* can activate caspase 3 is further strengthened by in vitro research on apoptotic cancer cell types. Additionally, medicarpin, maackiain, lupinalbin A, medioresinol, 8-o-methylretusin, biochanin A, isoliquiritigenin, coumestrol, and trigraecum are believed to be the nine compounds that best suit oral consumption. These substances are likely candidates for Caspase-3 and Bcl-2 protein activators in both pathways.

Competing interests

The authors declare no competing interests.

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