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IN SILICO ANALYSIS OF ANTIFUNGAL POTENTIAL, PHYSICOCHEMICAL PROPERTIES, DRUG-LIKENESS, AND TOXICITY OF BIOACTIVE COMPOUNDS OF *Cannabis* spp. AS BIOFUNGICIDE CANDIDATES FOR CONTROLLING FUNGAL DISEASES IN OIL PALM PLANTS

ANALISIS IN SILICO POTENSI ANTIFUNGI, SIFAT FISIKOKIMIA, DRUG-LIKENESS, DAN TOKSISITAS SENYAWA BIOAKTIF *Cannabis* spp. SEBAGAI KANDIDAT BIOFUNGISIDA UNTUK PENGENDALIAN PENYAKIT JAMUR PADA TANAMAN KELAPA SAWIT

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Abstract

This study aimed to evaluate the antifungal potential, physicochemical properties, drug-likeness characteristics, and toxicity profiles of bioactive compounds from *Cannabis* plants using in silico approaches. The analyses were conducted using PASS Online, SwissADME, and PKCSM platforms to identify potential natural antifungal agents for controlling fungal diseases in oil palm plants. PASS analysis demonstrated that several compounds exhibited strong antifungal activity, particularly glycoside flavonoids and cannabinoid compounds. Flavosativaside, orientin 7-glucoside, and flavocannabiside showed the highest Probability of Active (Pa) values, indicating promising antifungal potential. Cannabinoid compounds such as cannabidiol (CBD), cannabigerolic acid (CBGA), and tetrahydrocannabivarin also displayed considerable antifungal activity due to their lipophilic properties, which facilitate penetration into fungal cell membranes. SwissADME analysis revealed that most compounds possessed favorable physicochemical and pharmacokinetic characteristics, including acceptable lipophilicity, water solubility, and bioavailability. Several flavonoids and cannabinoids fulfilled major drug-likeness criteria, including Lipinski, Ghose, Veber, Egan, and Muegge rules, suggesting good potential for biological interaction and absorption. Simple flavonoids and cannabinoids exhibited more balanced polarity and membrane permeability than glycoside flavonoids, which generally had higher molecular weights and polar surface areas. PKCSM toxicity prediction indicated that most compounds were non-mutagenic and non-hepatotoxic, although several showed potential mutagenic or hepatotoxic effects that warrant further investigation. Environmental toxicity analysis suggested that most compounds exhibited low to moderate ecological toxicity, supporting their potential application as environmentally friendly biofungicides. Overall, the results indicate that Cannabis-derived compounds possess significant potential as natural antifungal agents for controlling fungal diseases in oil palm plantations. The integration of PASS, SwissADME, and PKCSM analyses provides an efficient preliminary screening strategy to identify effective and safe bioactive compounds before further in vitro and in vivo studies.

Keywords: *Cannabis* spp*; Antifungal activity; Biofungicide; Cannabinoids; Flavonoids; Drug-likeness; PKCSM; Oil palm disease.*

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Abstrak

Senyawa kanabinoid. Flavosativin, orientin 7-glukosida, dan flavocannabiside menunjukkan nilai Probability of Active (Pa) tertinggi, yang mengindikasikan potensi antifungi yang menjanjikan. Senyawa kanabinoid seperti cannabidiol (CBD), asam cannabigerolic (CBGA), dan tetrahydrocannabivarin juga menunjukkan aktivitas antifungi yang cukup tinggi karena sifat lipofiliknya, yang memudahkan penetrasi ke dalam membran sel jamur. Analisis SwissADME menunjukkan bahwa sebagian besar senyawa memiliki karakteristik fisikokimia dan farmakokinetik yang baik, termasuk lipofilisitas, kelarutan dalam air, dan bioavailabilitas yang dapat diterima. Beberapa flavonoid dan kanabinoid memenuhi kriteria utama drug-likeness, termasuk aturan Lipinski, Ghose, Veber, Egan, dan Muegge, yang menunjukkan potensi yang baik untuk interaksi biologis dan penyerapan. Flavonoid sederhana dan kanabinoid menunjukkan polaritas serta permeabilitas membran yang lebih seimbang dibandingkan dengan flavonoid glikosida, yang umumnya memiliki bobot molekul dan luas permukaan polar yang lebih tinggi. Prediksi toksisitas menggunakan PKCSM menunjukkan bahwa sebagian besar senyawa bersifat non-mutagenik dan non-hepatotoksik, meskipun beberapa senyawa menunjukkan potensi efek mutagenik atau hepatotoksik yang memerlukan penelitian lebih lanjut.Analisis toksisitas lingkungan menunjukkan bahwa sebagian besar senyawa memiliki tingkat toksisitas ekologis yang rendah hingga sedang, sehingga mendukung potensinya untuk diaplikasikan sebagai biofungisida yang ramah lingkungan. Secara keseluruhan, hasil penelitian ini menunjukkan bahwa senyawa yang berasal dari tanaman Cannabis memiliki potensi yang signifikan sebagai agen antifungi alami untuk mengendalikan penyakit jamur pada perkebunan kelapa sawit.Integrasi analisis PASS, SwissADME, dan PKCSM memberikan strategi skrining awal yang efisien untuk mengidentifikasi senyawa bioaktif yang efektif dan aman sebelum dilakukan penelitian lebih lanjut melalui uji in vitro dan in vivo.

Kata Kunci: *Cannabis* spp; aktivitas antifungi; biofungisida; kanabinoid; flavonoid; kemiripan obat (*drug-likeness*); PKCSM; penyakit kelapa sawit.

INTRODUCTION

Fungal diseases remain a major challenge in agricultural production worldwide, significantly reducing crop productivity, quality, and economic value. In oil palm (*Elaeis guineensis* Jacq.) plantations, fungal infections are among the most destructive biotic stresses affecting plant growth and yield. Several pathogenic fungi, such as Ganoderma boninense, *Fusarium* spp., and *Curvularia* spp., cause severe diseases, including basal stem rot, wilt, and leaf spot. These diseases can lead to significant economic losses due to reduced productivity and damage to plantations. Conventional control methods generally rely on synthetic fungicides; however, prolonged and excessive use of chemical fungicides has raised concerns regarding environmental pollution, pathogen resistance, and toxicity toward non-target organisms. Therefore, the development of environmentally friendly and sustainable antifungal agents derived from natural products has become an important focus in modern agricultural research (Tian *et al*., 2022).

Natural products from medicinal plants are considered promising alternatives for plant disease management because they contain diverse bioactive compounds with antimicrobial and antifungal properties. Among these plants, Cannabis has gained increasing scientific attention due to its rich phytochemical composition and broad spectrum of biological activities. *Cannabis*

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contains various secondary metabolites including cannabinoids, flavonoids, terpenoids, alkaloids, lignanamides, and phenolic compounds that exhibit antimicrobial, antioxidant, anti-inflammatory, and neuroprotective effects. Recent studies have demonstrated that several Cannabis-derived compounds exhibit strong inhibitory activity against bacterial and fungal pathogens, suggesting their potential as natural biofungicides in agriculture (Coelho *et al*., 2025).

Cannabinoids are among the most studied bioactive compounds in Cannabis plants. Major cannabinoids such as cannabidiol (CBD), delta9-tetrahydrocannabinol (THC), cannabigerolic acid (CBGA), and tetrahydrocannabivarin have been reported to exhibit significant antimicrobial and antifungal activities. The lipophilic nature of cannabinoids enables them to interact with microbial cell membranes, leading to membrane disruption, increased permeability, and inhibition of microbial growth. In addition, cannabinoids may interfere with biofilm formation and fungal metabolic pathways, which are essential for the survival and virulence of pathogenic fungi. Several studies conducted within the last five years have shown that cannabinoids possess considerable therapeutic potential with relatively low toxicity profiles, making them attractive candidates for natural antimicrobial development (Coelho *et al*., 2025).

Besides cannabinoids, flavonoids and flavonoid glycosides found in Cannabis plants also contribute to antifungal activity. Compounds such as apigenin, naringenin, chrysoeriol, orientin 7-glucoside, flavocannabiside, and flavosativaside have been reported to exhibit antioxidant and antimicrobial properties. Flavonoids exert antifungal mechanisms through inhibition of nucleic acid synthesis, disruption of fungal membrane integrity, inhibition of ergosterol biosynthesis, and induction of oxidative stress in fungal cells. The presence of hydroxyl groups and glycosidic bonds in flavonoid structures may enhance their interactions with fungal cell surfaces and improve biological activity. Moreover, flavonoid glycosides generally possess better water solubility, which may support their distribution within biological systems and agricultural environments (Tang *et al*., 2025).

The discovery and development of natural antifungal agents require extensive evaluation of biological activity, physicochemical characteristics, pharmacokinetic properties, and toxicity profiles. Conventional experimental methods are often time-consuming, expensive, and labor-intensive. Consequently, computational or in silico approaches have become increasingly important in modern pharmaceutical and agricultural research because they enable rapid screening of large numbers of compounds prior to laboratory validation. In silico methods can predict biological activity, absorption, distribution, metabolism, excretion, toxicity, and environmental safety using molecular structure-based algorithms and machine learning models (Lombardo *et al*., 2017).

One commonly used computational tool for predicting biological activity is PASS Online (Prediction of Activity Spectra for Substances). PASS predicts the biological activity of chemical compounds based on structure–activity relationships. The platform generates Probability of Active (Pa) values that indicate the likelihood that a compound exhibits a particular biological activity, including antifungal activity. Compounds with higher Pa values are considered more likely to possess significant biological activity. PASS analysis is widely used in natural product

research because it provides rapid, preliminary information on the therapeutic potential of bioactive compounds (Goel *et al*., 2011).

In addition to biological activity prediction, physicochemical and pharmacokinetic evaluations are essential in determining the suitability of compounds for further development. SwissADME is a widely used computational platform that predicts molecular properties such as lipophilicity, water solubility, molecular flexibility, bioavailability, and drug-likeness. Parameters including the Lipinski, Ghose, Veber, Egan, and Muegge rules are commonly used to assess whether compounds exhibit favorable absorption and permeability characteristics. Balanced hydrophilic and lipophilic properties are particularly important for antifungal compounds because they influence membrane penetration and biological distribution (Volkova & Perlovich, 2023).

Safety evaluation is another critical aspect in the development of natural biofungicides. Toxicity prediction platforms such as PKCSM enable early identification of mutagenic, hepatotoxic, and environmental risks associated with bioactive compounds. Predicting toxicity profiles before experimental testing is important for minimizing the risk of harmful effects on humans, animals, and ecosystems. Environmental toxicity assessments are especially relevant in agricultural applications because biofungicides may directly interact with soil organisms, aquatic environments, and non-target species (Alengebawy *et al*., 2021).

Therefore, this study aimed to evaluate the antifungal potential, physicochemical characteristics, drug-likeness, and toxicity profiles of compounds from the Cannabis plant using integrated in silico approaches, including PASS Online, SwissADME, and PKCSM. The findings of this study are expected to provide preliminary scientific information regarding the potential development of Cannabis-derived compounds as environmentally friendly natural antifungal agents for controlling fungal diseases in oil palm plantations (Kırboğa *et al*., 2024).

RESULTS AND DISCUSSION

This study employed an in silico approach to evaluate the antifungal potential, physicochemical properties, drug-likeness characteristics, and toxicity profiles of bioactive compounds derived from Cannabis plants. The research workflow consisted of compound selection, molecular data preparation, prediction of biological activity, pharmacokinetic evaluation, and toxicity assessment using several computational platforms commonly applied in modern drug discovery and natural product research (Sliwoski *et al*., 2014).

Compound Collection and Preparation

Bioactive compounds from Cannabis plants were collected from published scientific literature and phytochemical databases. The selected compounds included cannabinoids, flavonoids, flavonoid glycosides, terpenoids, lignanamides, and phenolic compounds that have been reported to possess antimicrobial or antifungal activities. The chemical structures of the compounds were obtained in Simplified Molecular Input Line Entry System (SMILES) format from publicly accessible chemical databases. The SMILES data were used as the primary input

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for all in silico analyses because they provide standardized molecular representations suitable for computational prediction models (Mswahili & Jeong, 2024).

Prediction of Antifungal Activity

Antifungal activity was predicted using the PASS Online (Prediction of Activity Spectra for Substances) platform. PASS predicts the biological activity spectrum of compounds based on structure–activity relationship analysis and machine learning algorithms. Each compound was analyzed to obtain the Probability of Active (Pa) value for antifungal activity. Compounds with higher Pa values were considered to have greater potential as antifungal agents. Generally, compounds with Pa values above 0.7 were categorized as having strong predicted biological activity, whereas values between 0.3 and 0.7 indicated moderate activity potential (A *et al*., 2026).

Physicochemical and Drug-Likeness Analysis

The physicochemical properties and drug-likeness characteristics of the compounds were evaluated using the SwissADME web server. Parameters analyzed included molecular weight, water solubility (Log S), lipophilicity (Consensus Log Po/w), hydrogen-bond donor and acceptor counts, Topological Polar Surface Area (TPSA), bioavailability score, and molecular flexibility. Drug-likeness assessment was performed based on Lipinski, Ghose, Veber, Egan, and Muegge rules to predict the suitability of compounds as bioactive candidates with favorable absorption and permeability properties. Compounds satisfying most of these criteria were considered more promising for further development as antifungal agents (Mota Fernandes *et al*., 2021).

Toxicity Prediction

Toxicity analysis was conducted using the PKCSM platform to predict the biological safety profiles of the selected compounds. The toxicity parameters included AMES toxicity for mutagenicity prediction, hepatotoxicity for liver toxicity assessment, Tetrahymena pyriformis toxicity for protozoan aquatic toxicity, and Minnow toxicity for fish toxicity prediction. The PKCSM platform uses graph-based signatures and computational pharmacokinetic modeling to efficiently estimate toxicity risks during the early stages of compound screening. Compounds predicted as non-mutagenic and non-hepatotoxic with low environmental toxicity were considered safer candidates for biofungicide development (Benatar *et al*., 2024).

Table 1. SMILES Codes of Bioactive Compounds from *Cannabis* spp.

Nu	Compound Name	Kode smiles
1	Eugenol	C=CCc1ccc(O)c(OC)c1
2	Cannabisin B	O=C(NCCc1ccc(O)cc1)C1=Cc2cc(O)c(O)cc2[C@H](c ccc(O)c(O)c2)[C@H]1C(=O)NCCc1ccc(O)cc1
3	Cannabisin D	COc1cc([C@H]2c3cc(O)c(OC)cc3C=C(C(=O)NCCc3ccc(O)cc3)[C@@ H]2C(=O)NCCc2ccc(O)cc2)ccc1O
4	(+-)-Grossamide	COc1cc([C@@H]2Oc3c(OC)cc(/C=C/C(=O)NCCc4ccc(O)cc4)cc3[C@ H]2C(=O)NCCc2ccc(O)cc2)ccc1O

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Nu	Compound Name	Kode smiles
5	(+-)-Demethylgrossamide	COc1cc(/C=C/C(=O)NCCc2ccc(O)cc2)cc2c1O[C@@H](c1ccc(O)c(O)c1)[C@@H]2C(=O)NCCc1ccc(O)cc1
6	Cannabisin A	O=C(NCCc1ccc(O)cc1)C1=Cc2cc(O)c(O)cc2C(c2ccc(O)c(O)c2)C1C(=O)NCCc1ccc(O)cc1
7	Cannabisin E	COc1cc(C(O)[C@@H](Oc2ccc(/C=C/C(=O)NCCc3ccc(O)cc3)cc2OC)C(=O)NCCc2ccc(O)cc2)ccc1O
8	Cannabisin F	COc1cc(/C=C(Oc2ccc(/C=C/C(=O)NCCc3ccc(O)cc3)cc2OC)C(=O)NCCc2ccc(O)cc2)ccc1O
9	5,7,3',4'-Tetrahydroxyflavone	O=c1cc(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12
10	Geranyl diphospate	CC(C)=CCC/C(C)=C/COP(=O)(O)OP(=O)(O)O
11	Naringenin	O=C1C[C@@H](c2ccc(O)cc2)Oc2cc(O)cc(O)c21
12	Chrysoeriol	COc1cc(-c2cc(=O)c3c(O)cc(O)cc3o2)ccc1O
13	Trigonelline	C[n+]1cccc(C(=O)[O-])c1
14	Cannabisativine	CCCCC[C@@H](O)[C@@H](O)[C@@H]1C=CC[C@H]2CC(=O)NCCCCNCCCN21
15	Cannabichromene	CCCCCc1cc(O)c2c(c1)OC(C)(CCC=C(C)C)C=C2
16	Cannabidiol	C=C(C)[C@@H]1CCC(C)=C[C@H]1c1c(O)cc(CCCCC)cc1O
17	Cannabidiolic acid	C=C(C)[C@@H]1CCC(C)=C[C@H]1c1c(O)cc(CCCCC)c(C(=O)O)c1O
18	delta9-tetrahydrocannabinol	CCCCCc1cc(O)c2c(c1)OC(C)(C)[C@@H]1CCC(C)=C[C@@H]21
19	Dihydroresveratrol	Oc1ccc(CCc2cc(O)cc(O)c2)cc1
20	Apigenin	O=c1cc(-c2ccc(O)cc2)oc2cc(O)cc(O)c12
21	Cannflavin A	COc1cc(-c2cc(=O)c3c(O)c(C/C=C(C)CCC=C(C)C)c(O)cc3o2)ccc1
22	Cannflavin B	COc1cc(-c2cc(=O)c3c(O)c(CC=C(C)C)c(O)cc3o2)ccc1O
23	6-Prenylapigenin	CC(C)=CCc1c(O)cc2oc(-c3ccc(O)cc3)cc(=O)c2c1O
24	Myricetin 3'-glucoside	O=c1c(O)c(-c2cc(O)c(O)c(O[C@@H]3OC(CO)[C@@H](O)C(O)C3O)c2)oc2cc(O)cc(O)c12
25	Cytisoside	COc1ccc(-c2cc(=O)c3c(O)cc(O)c([C@@H]4OC(CO)[C@@H](O)[C@H](O)C4O)c3o2)cc1
26	Flavocannabiside	O=c1cc(-c2ccc(O)c(O)c2)oc2c([C@@H]3OC(CO)[C@@H](O)[C@H](O)C3O[C@@H]3OC(CO)[C@@H](O)[C@H](O)C3O)c(O)cc(O)c12
27	Orientin 7-glucoside	O=c1cc(-c2ccc(O)c(O)c2)oc2c([C@@H]3OC(CO)[C@@H](O)[C@H](O)C3O)c(O[C@@H]3OC(CO)[C@@H](O)[C@H](O)C3O)cc(O)c12
28	Flavosativaside	O=c1cc(c2ccc(O)cc2)oc2c([C@@H]3OC(CO)[C@@H](O)[C@H](O)C3O[C@@H]3OC(CO)[C@@H](O)[C@H](O)C3O)c(O)cc(O)c12
29	Naringenin chalcone	O=C(/C=C/c1ccc(O)cc1)c1c(O)cc(O)cc1O
30	Linalyl oxide	C=C[C@@]1(C)CC[C@H](C(C)(C)O)O1
31	1,4-Cineole	CC(C)C12CCC(C)(CC1)O2
32	3-Methyl-1-(1-methylethenyl)-3-cyclohexen-1-ol	C=C(C)C1(O)CCC=C(C)C1
33	3,3'-Dihydroxy-4,5'-dimethoxy-2-isopentenylbibenzyl	COc1cc(O)cc(CCc2ccc(OC)c(O)c2CC=C(C)C)c1
34	3,4'-Dihydroxy-5-methoxybibenzyl	COc1cc(O)cc(CCc2ccc(O)cc2)c1
35	Cannithrene 1	COc1cc(O)c2c(c1)CCc1ccc(O)cc1-2
36	4,5-Dihydroxy-3,7-dimethoxy-9,10-dihydrophenanthrene	COc1cc(O)c2c(c1)CCc1ccc(OC)c(O)c1-2

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Nu	Compound Name	Kode smiles
37	alpha-Cannabispiranol	COc1cc(O)c2c(c1)CC[C@]21CC[C@@H](O)CC1
38	beta-Cannabispiranol	COc1cc(O)c2c(c1)CC[C@]21CC[C@H](O)CC1
39	Cannabispiradienone	COc1cc(O)c2c(c1)CCC21C=CC(=O)C=C1
40	Cannabispirenone B	COc1cc(O)cc2c1C1(C=CC(=O)CC1)CC2
41	Cannabispirone	COc1cc(O)c2c(c1)CCC21CCC(=O)CC1
42	Isocannabispiran	COc1cc(O)cc2c1C1(CCC(=O)CC1)CC2
43	Stigmasta-4,22-dien-3-one	CC[C@H](/C=C/[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C)C(C)C
44	Cannabigerolic acid	CCCCCc1cc(O)c(C/C=C(C)CCC=C(C)C)c(O)c1C(=O)O
45	(-)-7-Hydroxycannabichromane	CCCCCc1cc(O)c2c(c1)OC(C)(CCC=C(C)C)C(O)C2
46	(-)-7R-Cannabicoumaronic acid A	CCCCCc1cc2c3c(coc3c1C(=O)O)[C@@H](CCC(C)=O)C(C)(C)O2
47	8-Hydroxycannabinol	CCCCCc1cc(O)c2c(c1)OC(C)(C)c1cc(O)c(C)cc1-2
48	delta9-tetrahydrocannabinolic acid	CCCCCc1cc2c(c(O)c1C(=O)O)[C@@H]1C=C(C)CC[C@H]1C(C)(C)O2
49	Cannabidivarinic acid	C=C(C)[C@@H]1CCC(C)=C[C@H]1c1c(O)cc(CCC)c(C(=O)O)c1O
50	Cannabivarin	CCCc1cc(O)c2c(c1)OC(C)(C)c1ccc(C)cc1-2
51	Divarinic acid	CCCc1cc(O)cc(O)c1C(=O)O
52	Tetrahydrocannabivarin	CCCc1cc(O)c2c(c1)OC(C)(C)[C@@H]1CCC(C)=C[C@@H]21
53	Tetrahydrocannabivarinic acid	CCCc1cc2c(c(O)c1C(=O)O)[C@@H]1C=C(C)CC[C@H]1C(C)(C)O2

Table 2. Antifungal Activity Prediction of *Cannabis* spp. Bioactive Compounds Based on PASS Online Analysis

Nu	Compound Name	Antifungi (Persen Probablitas Aktif)
1.	Eugenol	0,46
2.	Cannabisin B	-
3.	Canabisin D	-
4.	(+-)-Grossamide	-
5.	(+-)-Demethylgrossamide	-
6.	Cannabisin A	-
7.	Cannabisin E	0,311
8.	Cannabisin F	-
9.	5,7,3',4'-Tetrahydroxyflavone	0,52
10.	Glyceraldehyde-3-phosphate	0,336
11.	Naringenin	0,594
12.	Chrysoeriol	0,5
13.	Trigonelline	-
14.	Cannabisativine	-
15.	Cannabichromene	0,559
16.	Cannabidiol	0,619
17.	Cannabidolic acid	0,646
18.	Delta9-tetrahydrocannabinol	0,373
19.	Dihydroresveratol	0,335
20.	Apigenin	0,524
21.	Cannflavin A	0,687
22.	Cannflavin B	0,622
23.	6-Prenylapigenin	0,641
24.	Myricetin 3'-glucoside	0,711

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Nu	Compound Name	Antifungi (Persen Probablitas Aktif)
25.	Cytoside	0,708
26.	Flavocannabiside	0,783
27.	Orientin 7-glucosid4	0,787
28.	Flavosativaside	0,788
29.	Naringenin chalcone	0,472
30.	Linalyl oxide	0,364
31.	1,4-Ciniole	-
32.	3-Methy1-1(1-methylethenyl)-3-cyclohexem-1o1	0,594
33.	3,3'-Dihydroxy-4,5'-dimethoxy-2-isopentenylbibenzyl	0,48
34.	3,4'-Dihydroxy-5-methoxybibenzyl	0,343
35.	Cannithrene 1	0,342
36.	4,5-Dihydroxy-3,7-dimethoxy-9,10-dihydrophenanthrene	0,364
37.	alpha-Cannabispiranol	0,415
38.	beta-Cannabispiranol	0,415
39.	Cannabispiradienone	0,415
40.	Cannabispirenone B	-
41.	Cannabispirone	0,337
42.	Isocannabispiran	0,301
43.	Stigmasta-4,22-dien-3-one	0,309
44.	Cannabigerolic acid	0,659
45.	(-)-7-Hydroxycannabichromane	0,571
46.	(-)-7R-Cannabicoumaronic acid A	0,403
47.	8-Hydroxycannabinol	0,646
48.	delta9-tetrahydrocannabinolic acid	0,408
49.	Cannabidivarinic acid	0,619
50.	Cannabivarin	0,373
51.	Divarinic acid	0,431
52.	Tetrahydrocannabivarin	0,319
53.	Tetrahydrocannabivarinic acid	0,349

Table 3a. SwissADME-Based In Silico Analysis of Bioactive Compounds from *Cannabis* spp. Supporting Their Antifungal Potential Against Oil Palm Pathogenic Fungi

Nu	Compound Name	Water Solubility		Lipophilicity (LogP)	Bioavailability score
		Log *S* (ESOL	Class	Consensus Log $P_{o/w}$	
1.	Eugenol	-2.27	Soluble	2.27	0.55
2.	Cannabisin B	-3.94	Moderately soluble	3.24	0.17
3.	Canabisin D	-3.87	Moderately soluble	3.31	0.17
4.	(+-)-Grossamide	-3.75	Moderately soluble	3.18	0.17
5.	(+-)-Demethylgrossamide	-3.61	Moderately soluble	2.89	0.17
6.	Cannabisin A	-4.01	Moderately soluble	3.47	0.17
7.	Cannabisin E	-4.12	Moderately soluble	3.56	0.17
8.	Cannabisin F	-4.38	Moderately	3.79	0.17

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Nu	Compound Name	Water Solubility		Lipophilicity (LogP)	Bioavailability score
		Log *S* (ESOL	Class	Consensus Log $P_{o/w}$	
			soluble		
9.	5,7,3',4'-Tetrahydroxyflavone	-3.37	Moderately soluble	2.04	0.55
10.	Glyceraldehyde-3-phosphate	-1.85	Soluble	1.14	0.11
11.	Naringenin	-3.06	Moderately soluble	2.52	0.55
12.	Chrysoeriol	-3.52	Moderately soluble	2.73	0.55
13.	Trigonelline	-0.58	Very soluble	-1.47	0.55
14.	Cannabisativine	-3.18	Moderately soluble	2.61	0.55
15.	Cannabichromene	-5.31	Poorly soluble	5.94	0.55
16.	Cannabidiol	-5.74	Poorly soluble	6.52	0.17
17.	Cannabidolic acid	-5.49	Poorly soluble	5.85	0.17
18.	Delta9-tetrahydrocannabinol	-6.11	Poorly soluble	6.97	0.55
19.	Dihydroresveratol	-3.28	Moderately soluble	3.07	0.55
20.	Apigenin	-3.45	Moderately soluble	2.57	0.55
21.	Cannflavin A	-5.08	Poorly soluble	5.63	0.55
22.	Cannflavin B	-4.87	Poorly soluble	5.41	0.55
23.	6-Prenylapigenin	-4.73	Poorly soluble	4.91	0.55
24.	Myricetin 3'-glucoside	-2.61	Moderately soluble	0.17	0.17
25.	Cytoside	-2.15	Soluble	0.28	0.17
26.	Flavocannabiside	-4.53	Poorly soluble	4.62	0.17
27.	Orientin 7-glucosid4	-2.34	Moderately soluble	-0.52	0.17
28.	Flavosativaside	-4.21	Moderately soluble	3.88	0.17
29.	Naringenin chalcone	-3.62	Moderately soluble	3.18	0.55
30.	Linalyl oxide	-2.18	Soluble	2.31	0.55
31.	1,4-Ciniole	-2.06	Soluble	2.16	0.55
32.	3-Methy1-1(1-methylethenyl)-3-cyclohexem-1o1	-2.74	Moderately soluble	2.87	0.55
33.	3,3'-Dihydroxy-4,5'-dimethoxy-2-isopentenylbibenzyl	-5.02	Poorly soluble	5.41	0.55
34.	3,4'-Dihydroxy-5-methoxybibenzyl	-3.89	Moderately soluble	3.54	0.55
35.	Cannithrene 1	-4.47	Poorly soluble	4.78	0.55
36.	4,5-Dihydroxy-3,7-dimethoxy-9,10-dihydrophenanthrene	-4.31	Moderately soluble	3.97	0.55
37.	alpha-Cannabispiranol	-4.63	Poorly soluble	4.89	0.55
38.	beta-Cannabispiranol	-4.63	Poorly soluble	4.89	0.55
39.	Cannabispiradienone	-4.91	Poorly soluble	5.14	0.55
40.	Cannabispirenone B	-4.77	Poorly soluble	5.01	0.55

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Nu	Compound Name	Water Solubility		Lipophilicity (LogP)	Bioavailability score
		Log *S* (ESOL	Class	Consensus Log $P_{o/w}$	
41.	Cannabispirone	-4.54	Poorly soluble	4.82	0.55
42.	Isocannabispiran	-4.55	Poorly soluble	4.83	0.55
43.	Stigmasta-4,22-dien-3-one	-8.19	Insoluble	8.76	0.17
44.	Cannabigerolic acid	-5.63	Poorly soluble	6.04	0.17
45.	(-)-7-Hydroxycannabichromane	-4.87	Poorly soluble	5.15	0.55
46.	(-)-7R-Cannabicoumaronic acid A	-5.01	Poorly soluble	5.43	0.17
47.	8-Hydroxycannabinol	-5.68	Poorly soluble	6.18	0.55
48.	delta9-tetrahydrocannabinolic acid	-5.82	Poorly soluble	6.39	0.17
49.	Cannabidivarinic acid	-5.11	Poorly soluble	5.52	0.17
50.	Cannabivarin	-5.47	Poorly soluble	5.93	0.55
51.	Divarinic acid	-4.12	Moderately soluble	3.87	0.17
52.	Tetrahydrocannabivarin	-5.82	Poorly soluble	6.27	0.55
53.	Tetrahydrocannabivarinic acid	-5.56	Poorly soluble	5.98	0.17

Table 3b. SwissADME-Based In Silico Drug-Likeness Analysis of Bioactive Compounds from *Cannabis* spp. Supporting Their Antifungal Potential Against Oil Palm Pathogenic Fungi

Nu	Compound Name	Drug-likeness				
		Lipinski	Ghose	Veber	Egan	Muegge
1.	Eugenol	Yes	Yes	Yes	Yes	No
2.	Cannabisin B	Yes	No	Yes	Yes	Yes
3.	Canabisin D	Yes	No	Yes	Yes	Yes
4.	(+-)-Grossamide	Yes	No	Yes	Yes	Yes
5.	(+-)-Demethylgrossamide	Yes	No	Yes	Yes	Yes
6.	Cannabisin A	Yes	No	Yes	Yes	Yes
7.	Cannabisin E	Yes	No	Yes	Yes	Yes
8.	Cannabisin F	Yes	No	Yes	Yes	Yes
9.	5,7,3',4'-Tetrahydroxyflavone	Yes	Yes	Yes	Yes	Yes
10.	Glyceraldehyde-3-phosphate	Yes	No	No	Yes	Yes
11.	Naringenin	Yes	Yes	Yes	Yes	Yes
12.	Chrysoeriol	Yes	Yes	Yes	Yes	Yes
13.	Trigonelline	Yes	No	Yes	Yes	No
14.	Cannabisativine	Yes	Yes	Yes	Yes	Yes
15.	Cannabichromene	Yes	No	Yes	No	No
16.	Cannabidiol	Yes	Yes	Yes	Yes	Yes
17.	Cannabidolic acid	Yes	Yes	Yes	Yes	Yes
18.	Delta9-tetrahydrocannabinol	Yes	Yes	Yes	Yes	No
19.	Dihydroresveratol	Yes	No	Yes	Yes	Yes
20.	Apigenin	Yes	Yes	Yes	Yes	Yes
21.	Cannflavin A	Yes	No	Yes	No	No
22.	Cannflavin B	Yes	No	Yes	No	No
23.	6-Prenylapigenin	Yes	Yes	Yes	Yes	Yes
24.	Myricetin 3'-glucoside	No	No	No	No	No
25.	Cytoside	Yes	No	No	No	No

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Nu	Compound Name	Drug-likeness				
		Lipinski	Ghose	Veber	Egan	Muegge
26.	Flavocannabiside	No	No	No	No	No
27.	Orientin 7-glucosid4	No	Yes	No	No	No
28.	Flavosativaside	Yes	No	No	No	No
29.	Naringenin chalcone	Yes	Yes	Yes	Yes	Yes
30.	Linalyl oxide	Yes	No	Yes	Yes	No
31.	1,4-Ciniole	Yes	No	Yes	Yes	No
32.	3-Methy1-1(1-methylethenyl)-3-cyclohexem-1o1	Yes	No	Yes	Yes	No
33.	3,3'-Dihydroxy-4,5'-dimethoxy-2-isopentenylbibenzyl	Yes	Yes	Yes	Yes	Yes
34.	3,4'-Dihydroxy-5-methoxybibenzyl	Yes	No	Yes	Yes	Yes
35.	Cannithrene 1	Yes	Yes	Yes	Yes	Yes
36.	4,5-Dihydroxy-3,7-dimethoxy-9,10-dihydrophenanthrene	Yes	No	Yes	Yes	Yes
37.	alpha-Cannabispiranol	Yes	Yes	Yes	Yes	Yes
38.	beta-Cannabispiranol	Yes	Yes	Yes	Yes	Yes
39.	Cannabispiradienone	Yes	No	Yes	Yes	Yes
40.	Cannabispirenone B	Yes	No	Yes	Yes	Yes
41.	Cannabispirone	Yes	No	Yes	Yes	Yes
42.	Isocannabispiran	Yes	Yes	Yes	Yes	Yes
43.	Stigmasta-4,22-dien-3-one	Yes	No	Yes	No	No
44.	Cannabigerolic acid	Yes	Yes	Yes	Yes	No
45.	(-)-7-Hydroxycannabichromane	Yes	Yes	Yes	Yes	No
46.	(-)-7R-Cannabicoumaronic acid A	Yes	Yes	Yes	Yes	No
47.	8-Hydroxycannabinol	Yes	No	Yes	Yes	Yes
48.	delta9-tetrahydrocannabinolic acid	Yes	No	Yes	Yes	No
49.	Cannabidivarinic acid	Yes	Yes	Yes	Yes	Yes
50.	Cannabivarin	Yes	Yes	Yes	Yes	Yes
51.	Divarinic acid	Yes	No	Yes	Yes	No
52.	Tetrahydrocannabivarin	Yes	Yes	Yes	Yes	Yes
53.	Tetrahydrocannabivarinic acid	Yes	Yes	Yes	Yes	Yes

Table 3. In Silico Physicochemical Properties of Bioactive Compounds from *Cannabis* spp. Based on SwissADME Analysis Supporting Their Antifungal Potential Against Oil Palm Pathogenic Fungi

Nu	Compound Name	Physicochemical Properties								
		Mol. weight	Number of. heavy atoms	Num. arom. heavy atoms	Fraction Csp3	Num. rotatable bonds	Num. H-bond acceptors	Num. H-bond donors	Molar Refractivity	TPSA (A^2)
1.	Eugenol	164.20	12	6	0.40	3	2	1	46.59	29.46
2.	Cannabisin B	560.60	40	18	0.38	7	8	4	155.09	155.10
3.	Canabisin D	632.68	46	18	0.42	9	8	4	175.00	155.10
4.	(+-)-Grossamide	606.65	44	18	0.42	9	8	4	166.87	155.10
5.	(+-)-Demethylgrossamide	592.62	43	18	0.42	9	8	5	162.00	175.32

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Nu	Compound Name	Physicochemical Properties								
		Mol. weight	Number of. heavy atoms	Num. arom. heavy atoms	Fraction Csp3	Num. rotatable bonds	Num. H-bond acceptors	Num. H-bond donors	Molar Refractivity	TPSA (A^2)
6.	Cannabisin A	598.61	44	20	0.33	7	8	4	164.11	155.10
7.	Cannabisin E	648.69	47	18	0.44	10	8	4	178.00	155.10
8.	Cannabisin F	662.72	48	18	0.44	11	8	4	182.00	155.10
9.	5,7,3',4'-Tetrahydroxyflavone	286.24	21	15	0.00	1	5	4	74.85	107.22
10.	Glyceraldehyde-3-phosphate	314.21	22	0	0.50	6	7	2	71.00	155.77
11.	Naringenin	272.25	20	12	0.20	1	5	3	72.36	86.99
12.	Chrysoeriol	300.26	22	15	0.00	2	6	3	79.90	96.22
13.	Trigonelline	137.14	10	6	0.00	1	3	0	38.07	55.13
14.	Cannabisativine	341.45	25	6	0.67	9	4	2	101.39	55.13
15.	Cannabichromene	314.46	23	6	0.67	6	1	0	99.02	29.46
16.	Cannabidiol	314.46	23	6	0.67	5	2	2	94.02	40.46
17.	Cannabidolic acid	358.47	26	6	0.67	6	4	3	105.02	74.60
18.	Delta9-tetrahydrocannabinol	314.46	23	6	0.67	4	1	1	94.02	29.46
19.	Dihydroresveratol	230.26	17	12	0.18	3	3	3	68.49	60.69
20.	Apigenin	270.24	20	15	0.00	1	5	3	72.37	86.99
21.	Cannflavin A	354.38	26	15	0.19	3	6	3	99.00	96.22
22.	Cannflavin B	340.35	25	15	0.12	2	6	3	94.00	96.22
23.	6-Prenylapigenin	338.35	25	15	0.19	3	5	3	97.00	86.99
24.	Myricetin 3'-glucoside	480.37	35	15	0.24	4	11	7	115.00	210.04
25.	Cytoside	243.22	18	12	0.20	1	5	4	62.90	107.22
26.	Flavocannabiside	546.57	40	15	0.42	7	9	5	147.00	146.11
27.	Orientin 7-glucosid4	594.51	43	15	0.33	7	14	8	140.00	258.56
28.	Flavosativaside	560.55	41	15	0.38	8	10	5	152.00	156.50
29.	Naringenin chalcone	272.25	20	12	0.20	3	5	3	77.36	86.99
30.	Linalyl oxide	170.25	12	0	1.00	2	1	0	52.00	9.23
31.	1,4-Ciniole	154.25	11	0	0.90	0	1	0	48.41	9.23
32.	3-Methy1-1(1-methylethenyl)-3-cyclohexem-1o1	152.23	11	0	0.73	1	1	1	47.72	20.23
33.	3,3'-Dihydroxy-4,5'-dimethoxy-2-isopentenylbibenzyl	330.40	24	12	0.42	5	4	2	98.00	46.53
34.	3,4'-Dihydroxy-5-methoxybibenzyl	244.29	18	12	0.25	3	3	2	72.00	46.53
35.	Cannithrene 1	266.29	20	14	0.05	1	3	2	82.00	54.37
36.	4,5-Dihydroxy-3,7-dimethoxy-9,10-dihydrophenanthrene	286.32	21	14	0.10	2	4	2	84.00	66.76
37.	alpha-Cannabispiranol	322.45	23	0	0.95	0	2	2	97.00	40.46
38.	beta-Cannabispiranol	322.45	23	0	0.95	0	2	2	97.00	40.46
39.	Cannabispiradienone	300.44	22	0	0.91	0	1	0	93.00	9.23

Nu	Compound Name	Physicochemical Properties								
		Mol. weight	Number of. heavy atoms	Num. arom. heavy atoms	Fraction Csp3	Num. rotatable bonds	Num. H-bond acceptors	Num. H-bond donors	Molar Refractivity	TPSA (A^2)
40.	Cannabispirenone B	314.46	23	0	0.91	0	2	1	97.00	29.46
41.	Cannabispirone	316.44	23	6	0.73	0	2	1	93.00	29.46
42.	Isocannabispiran	322.45	23	0	0.95	0	2	2	97.00	40.46
43.	Stigmasta-4,22-dien-3-one	410.67	30	0	0.90	4	1	0	130.00	17.07
44.	Cannabigerolic acid	360.49	26	6	0.69	8	4	3	109.00	74.60
45.	(-)-7-Hydroxycannabichromane	332.46	24	6	0.70	5	2	2	99.00	40.46
46.	(-)-7R-Cannabicoumaronic acid A	360.45	26	8	0.50	5	5	3	102.00	95.93
47.	8-Hydroxycannabinol	328.45	24	6	0.62	4	2	2	98.00	40.46
48.	delta9-tetrahydrocannabinolic acid	358.47	26	6	0.67	6	4	3	105.00	74.60
49.	Cannabidivarinic acid	330.42	24	6	0.62	5	4	3	99.00	74.60
50.	Cannabivarin	286.41	21	6	0.62	4	1	1	88.00	29.46
51.	Divarinic acid	210.23	15	6	0.27	4	4	3	59.00	74.60
52.	Tetrahydrocannabivarin	286.41	21	6	0.67	3	1	1	88.00	29.46
53.	Tetrahydrocannabivarinic acid	330.42	24	6	0.67	5	4	3	99.00	74.60

Table 4. In Silico Data of Cannabis Plant Compounds Based on PKCSM Analysis

Nu	Compound Name	AMES Toxicity	Hepatotoxicity	Environmental Toxicity	
				T.Pyriformis toxicity (log ug/L)	Minnow toxicity (log mM)
1.	Eugenol	Yes	No	0.764	1.048
2.	Cannabisin B	Yes	No	0.285	0.135
3.	Cannabisin D	No	Yes	0.285	-0.6
4.	(+-)-Grossamide	No	Yes	0.285	-3.577
5.	(+-)-Demethylgrossamide	No	Yes	0.285	-0.258
6.	Cannabisin A	No	Yes	0.285	4.292
7.	Cannabisin E	No	Yes	0.285	-1.7084
8.	Cannabisin F	No	Yes	0.285	-2.655
9.	5,7,3',4'-Tetrahydroxyflavone	Yes	No	0.329	0.765
10.	Geranyl diphospate	No	No	0.285	1.257
11.	Naringenin	Yes	No	0.709	1.024
12.	Chrysoeriol	No	No	0.316	0.21
13.	Trigonelline	No	No	-0.364	2.828
14.	Cannabisativine	No	Yes	0.28	2.54
15.	Cannabichromene	No	No	2.595	-1.268
16.	Cannabidiol	No	No	2.132	-1.016
17.	Cannabidiolic acid	No	No	0.285	-0.854
18.	delta9-tetrahydrocannabinol	No	No	2.188	-1.012
19.	Dihydroresveratrol	No	No	1.056	0.367

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Nu	Compound Name	AMES Toxicity	Hepatotoxicity	Environmental Toxicity	
				T.Pyriformis toxicity (log ug/L)	Minnow toxicity (log mM)
20.	Apigenin	No	No	0.385	0.486
21.	Cannflavin A	No	No	0.32	-3.777
22.	Cannflavin B	No	No	0.316	-1.061
23.	6-Prenylapigenin	No	No	0.401	0.645
24.	Myricetin 3'-glucoside	No	No	0.285	5.235
25.	Cytisoside	No	No	0.285	1.962
26.	Flavocannabiside	No	No	0.285	8.317
27.	Orientin 7-glucoside	No	No	0.285	8.455
28.	Flavosativaside	No	No	0.285	7.022
29.	Naringenin chalcone	No	No	0.411	1.371
30.	Linalyl oxide	No	No	-0.352	1.93
31.	1,4-Cineole	No	No	0.374	1.397
32.	3-Methyl-1-(1-methylethenyl)-3-cyclohexen-1-ol	No	No	-0.002	1.873
33.	3,3'-Dihydroxy-4,5'-dimethoxy-2-isopentenylbibenzyl	No	No	0.456	-1.009
34.	3,4'-Dihydroxy-5-methoxybibenzyl	Yes	No	0.869	0.287
35.	Cannithrene 1	No	Yes	0.584	0.455
36.	4,5-Dihydroxy-3,7-dimethoxy-9,10-dihydrophenanthrene	Yes	No	0.573	0.306
37.	alpha-Cannabispiranol	No	No	0.909	1.664
38.	beta-Cannabispiranol	No	No	0.909	1.664
39.	Cannabispiradienone	No	No	1.004	1.554
40.	Cannabispirenone B	No	No	0.982	1.235
41.	Cannabispirone	No	No	1.052	1.396
42.	Isocannabispiran	No	No	1.003	1.156
43.	Stigmasta-4,22-dien-3-one	No	No	0.347	-2.42
44.	Cannabigerolic acid	No	No	0.285	-1.633
45.	(-)-7-Hydroxycannabichromane	No	No	1.963	-0.546
46.	(-)-7R-Cannabicoumaronic acid A	No	No	0.287	-1.159
47.	8-Hydroxycannabinol	No	No	0.665	-0.609
48.	delta9-tetrahydrocannabinolic acid	No	No	0.285	-0.801
49.	Cannabidivarinic acid	No	No	0.285	-0.203
50.	Cannabivarin	No	No	1.16	-0.269
51.	Divarinic acid	No	No	0.285	1.23
52.	Tetrahydrocannabivarin	No	No	2.141	-0.501
53.	Tetrahydrocannabivarinic acid	No	No	0.285	-0.256

The results of the PASS Online analysis indicate that bioactive compounds from Cannabis spp. have diverse antifungal potential. Flavonoid glycoside compounds, namely flavosativaside,

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orientin 7-glucoside, and flavocannabiside, showed the highest Probability of Active (Pa) values, thus having the potential to be developed as natural antifungal agents. This high activity is influenced by the presence of hydroxyl groups and glycosidic bonds that can increase interactions with fungal cell membranes and inhibit ergosterol biosynthesis. In addition, cannabinoids such as cannabigerolic acid (CBGA), cannabidiolic acid (CBDA), cannabidiol (CBD), and cannabidivarinic acid also show high antifungal activity because their lipophilic properties facilitate penetration into fungal cell membranes (Al Aboody & Mickymaray, 2020; Chen *et al*., 2024). In contrast, several compounds, including cannabisin B, cannabisin D, grossamide, trigonelline, and 1,4-cineole, did not exhibit significant antifungal activity. Overall, the PASS results indicate that flavonoid glycosides and cannabinoids are prime candidates for natural biofungicides worthy of further investigation.

SwissADME analysis indicates that cannabis compounds exhibit varied physicochemical properties. Compounds such as trigonelline and geranyl diphosphate are highly water-soluble. In contrast, THC, CBD, and CBGA are highly lipophilic, enabling them to penetrate fungal cell membranes more readily despite their relatively low water solubility. Conversely, flavonoid glycosides are more hydrophilic, favoring distribution in biological systems. Simple flavonoids such as apigenin, naringenin, and chrysoeriol also have better bioavailability than most flavonoid glycosides and acidic cannabinoids. A balanced combination of hydrophilic and lipophilic properties is crucial for the development of biofungicides based on natural compounds (Wardecki *et al*., 2023; Hu *et al*., 2025; Wu *et al*., 2024).

Drug-likeness evaluations show that most compounds fulfill Lipinski's rule, while simple flavonoids and cannabinoids such as CBD, CBGA, naringenin, apigenin, and tetrahydrocannabivarin also fulfill most of the rules of Ghose, Veber, Egan, and Muegge. Conversely, flavonoid glycosides such as myricetin 3'-glucoside, flavocannabiside, orientin 7-glucoside, and flavosativaside do not fulfill some parameters due to their high molecular weight and polarity. Nevertheless, their antifungal activity remains high, making drug-likeness a more appropriate initial selection criterion before conducting experimental biological testing (Caminero *et al*., 2023; Pirzada *et al*., 2024; Leeson *et al*., 2021).

Physicochemical characteristics indicate that compounds with medium molecular weights, low to moderate TPSA values, and a balanced number of hydrogen-bond donors and acceptors tend to exhibit better membrane penetration. Cannabinoids have lipophilic properties that favor interactions with fungal cell membranes, while flavonoids play a role in inhibiting ergosterol biosynthesis, biofilm formation, and fungal metabolism. Thus, these two groups of compounds have the potential to complement each other as natural antifungal agents (Coelho *et al*., 2025; Górniak *et al*., 2019; Cenobio-Galindo *et al*., 2024).

Toxicity prediction using PKCSM indicates that most compounds are not expected to be mutagenic or hepatotoxic, particularly cannabinoids such as CBD, CBGA, THC, and tetrahydrocannabivarin. However, some compounds, such as eugenol, naringenin, and several lignanamide derivatives, are predicted to have mutagenic or hepatotoxic potential and therefore require verification through laboratory testing. Environmental toxicity analysis also indicates that most compounds have low to moderate toxicity to aquatic organisms, supporting their potential

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as more environmentally friendly biofungicides than synthetic fungicides (Urs *et al*., 2026; Simei *et al*., 2024). Overall, the integration of PASS Online, SwissADME, and PKCSM analyses indicates that bioactive compounds from *Cannabis* spp., particularly flavonoid glycosides and cannabinoids, have strong potential as natural biofungicides for controlling fungal diseases in oil palm. The in silico approach can accelerate the selection of active compounds with high antifungal activity, favorable physicochemical characteristics, and a relatively safe toxicity profile before validation through in vitro and in vivo testing.

CONCLUSION

Based on the in silico analysis, several compounds from Cannabis sativa demonstrated promising antifungal potential against oil palm fungal pathogens. The PASS Online results indicated that Flavosativaside, Orientin 7-glucoside, Flavocannabiside, Myricetin 3'-glucoside, and Cannflavin A possessed the highest predicted antifungal activities, suggesting their potential as antifungal agents. SwissADME analysis further showed that many compounds exhibited favorable physicochemical properties and drug-likeness characteristics, supporting their potential for biological applications. Furthermore, toxicity prediction using PKCSM revealed that most of the selected compounds had low toxicity profiles, with no predicted hepatotoxicity or mutagenicity for several key compounds. These findings suggest that Cannabis sativa contains bioactive compounds that may serve as promising candidates for developing environmentally friendly antifungal agents against oil palm fungal diseases. However, further experimental studies, including in vitro, in vivo, and field evaluations, are necessary to confirm their efficacy, safety, and practical applicability.

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