Standard Seed Corporation

FEBRUARY 17th 2025

Artificial Intelligence Chemical Report

Cannflavin A

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Global Botanical Artificial Intelligence System (GBAIS)

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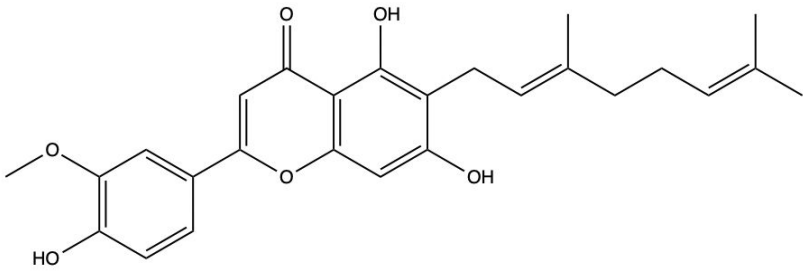
Chemical Profile



Global-Chem Name: Cannflavin A

SMILES:

CC(=CCC/C(=C/CC1=C(C2=C(C=C1O)OC(=CC2=O)C3=CC(=C(C=C3)O)OC)O)/C)C

Molecular Weight: 436.504

Calculated ALogP: 5.82

Calculated $LogD_{7,4}$: 4.82

LogP (Crippen Method): 5.821

Calculated Acidic PKa: 6.39

Hydrogen Bond Acceptors: 6

Hydrogen Bond Donors: 3

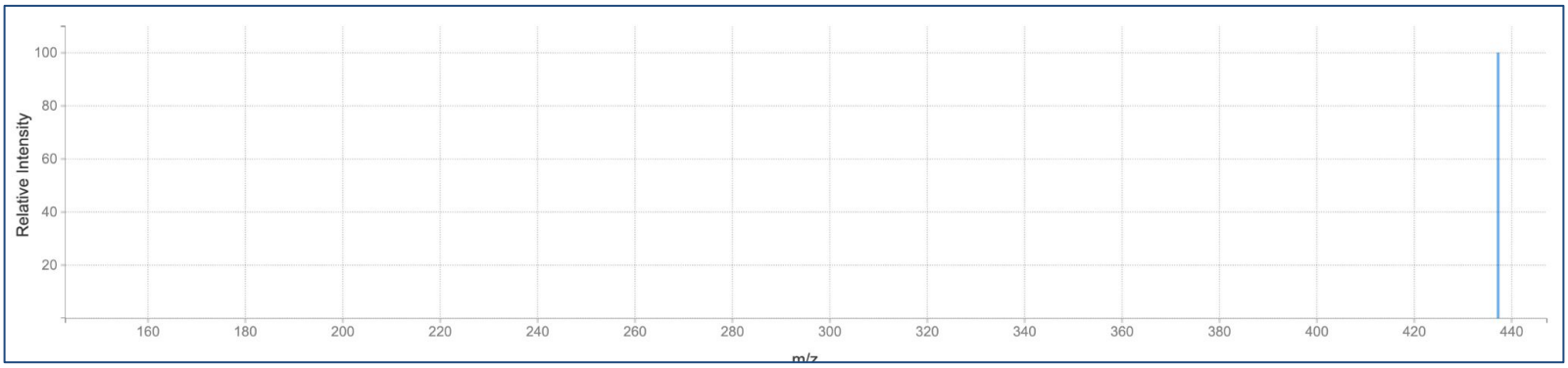
Topological Polar Surface Area: 100.130

Drug-likeness QED Weight: 0.40

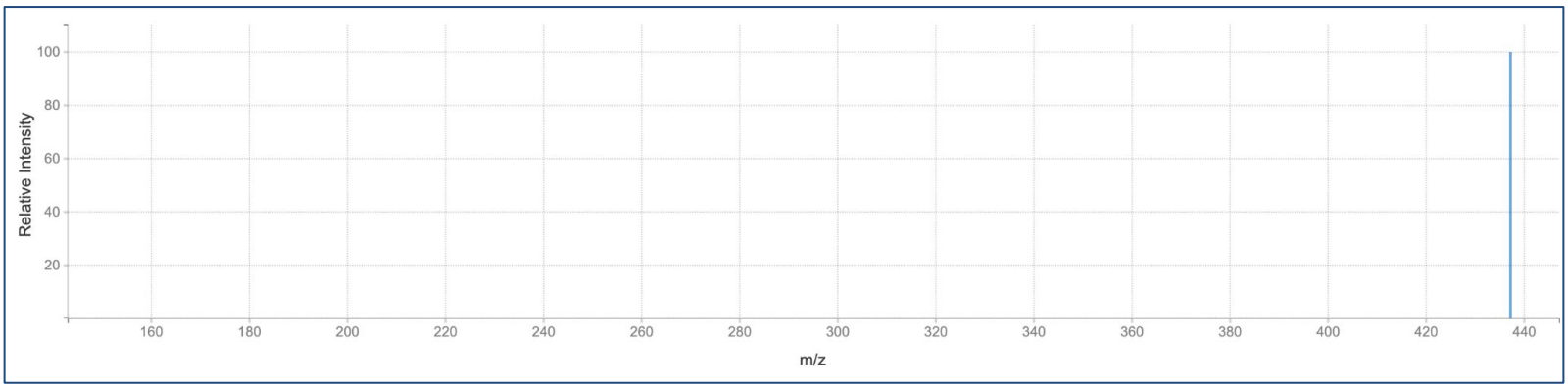
Compound Characterization: Digital Twin Mass Spectrometry

Spectra Type: Electrospray Ionization (ESI)
Ion Mode: Positive
Adduct Type: [M+H]+
Digital Twin Instrument: Agilent 6510 Q-TOF
Blue lines are the parent mass fragment. **Red** lines are fragments.

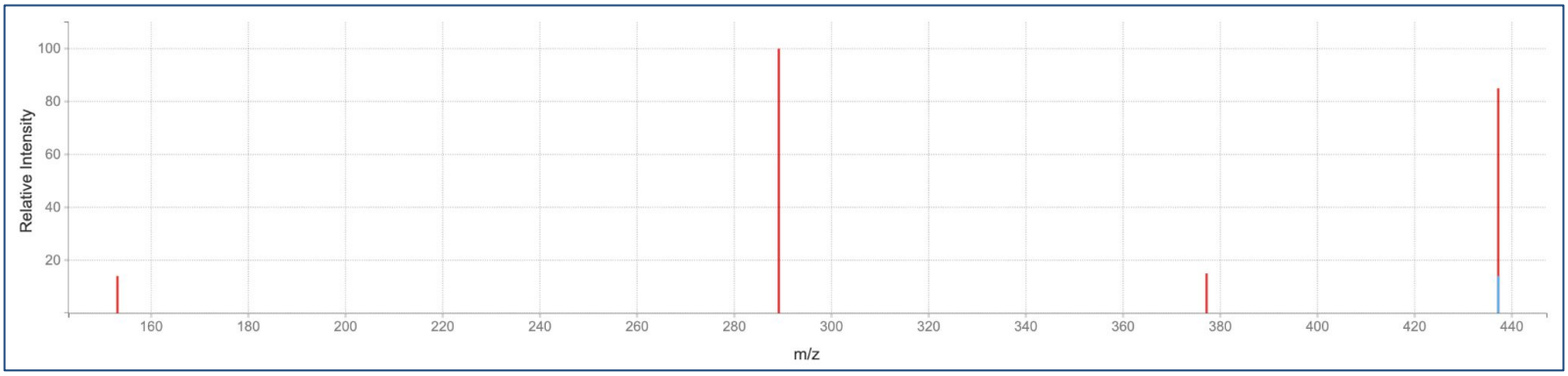
Predicted Low Energy MsMs Spectrum (10V), [M+H]+



Predicted Medium Energy MsMs Spectrum (20V), [M+H]+

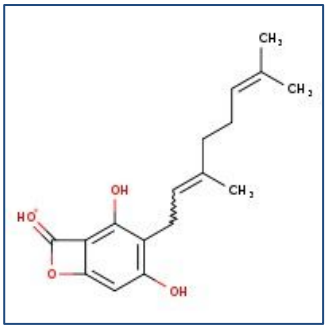


Predicted High Energy MsMs Spectrum (40V), [M+H]+



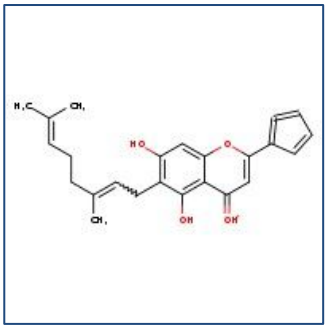
Compound Characterization: Mass Spectrometry (Major/Minor Fragments)

Major

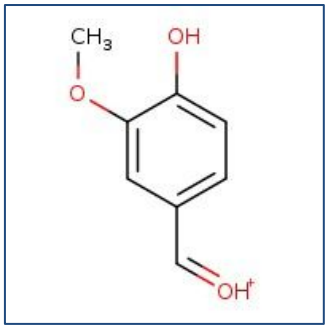


Mass: 289.143

Minor

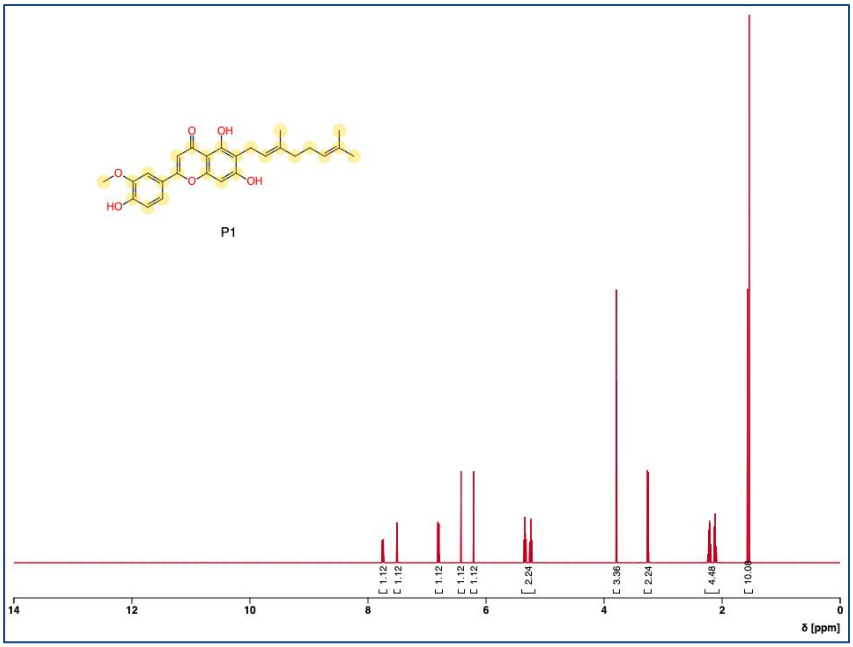


Mass: 377.174

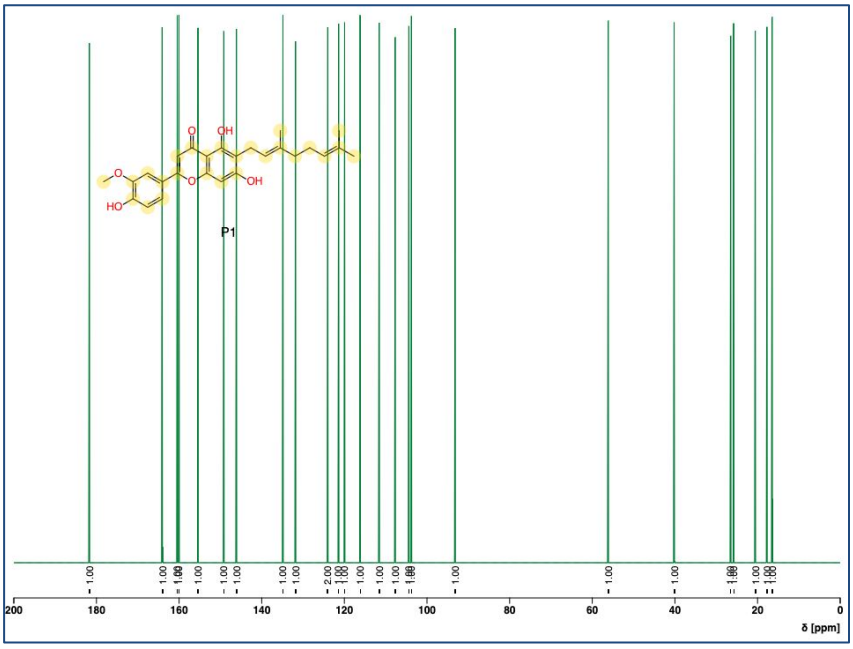


Mass: 153.054

Compound Characterization: Digital Twin 400 MHz Nuclear Magnetic Resonance Spectroscopy



1H NMR (400 MHz): δ 1.49-1.62 (10H, 1.54 (s), 1.54 (s), 1.57 (s)), 2.05-2.29 (4H, 2.12 (t, J = 7.43 Hz), 2.22 (td, J = 7.43, 7.16 Hz)), 3.26 (2H, d, J = 6.73 Hz), 3.79 (3H, s), 5.17-5.40 (2H, 5.24 (t, J = 7.16 Hz), 5.34 (t, J = 6.73 Hz)), 6.21 (1H, s), 6.42 (1H, s), 6.80 (1H, dd, J = 8.43, 0.45 Hz), 7.50 (1H, dd, J = 1.72, 0.45 Hz), 7.75 (1H, dd, J = 8.43, 1.72 Hz).



13C NMR (101 MHz): δ 16.40 (1C, s), 17.68 (1C, s), 20.50 (1C, s), 25.70 (1C, s), 26.50 (1C, s), 40.10 (1C, s), 56.11 (1C, s), 93.20 (1C, s), 103.70 (1C, s), 104.38 (1C, s), 107.70 (1C, s), 111.50 (1C, s), 116.10 (1C, s), 119.90 (1C, s), 121.40 (1C, s), 123.95-124.15 (2C, 124.00 (s), 124.10 (s)), 131.80 (1C, s), 134.85 (1C, s), 146.10 (1C, s), 149.10 (1C, s), 155.40 (1C, s), 160.00 (1C, s), 160.40 (1C, s), 164.00 (1C, s), 181.70 (1C, s).

Solubility Solvent Prediction

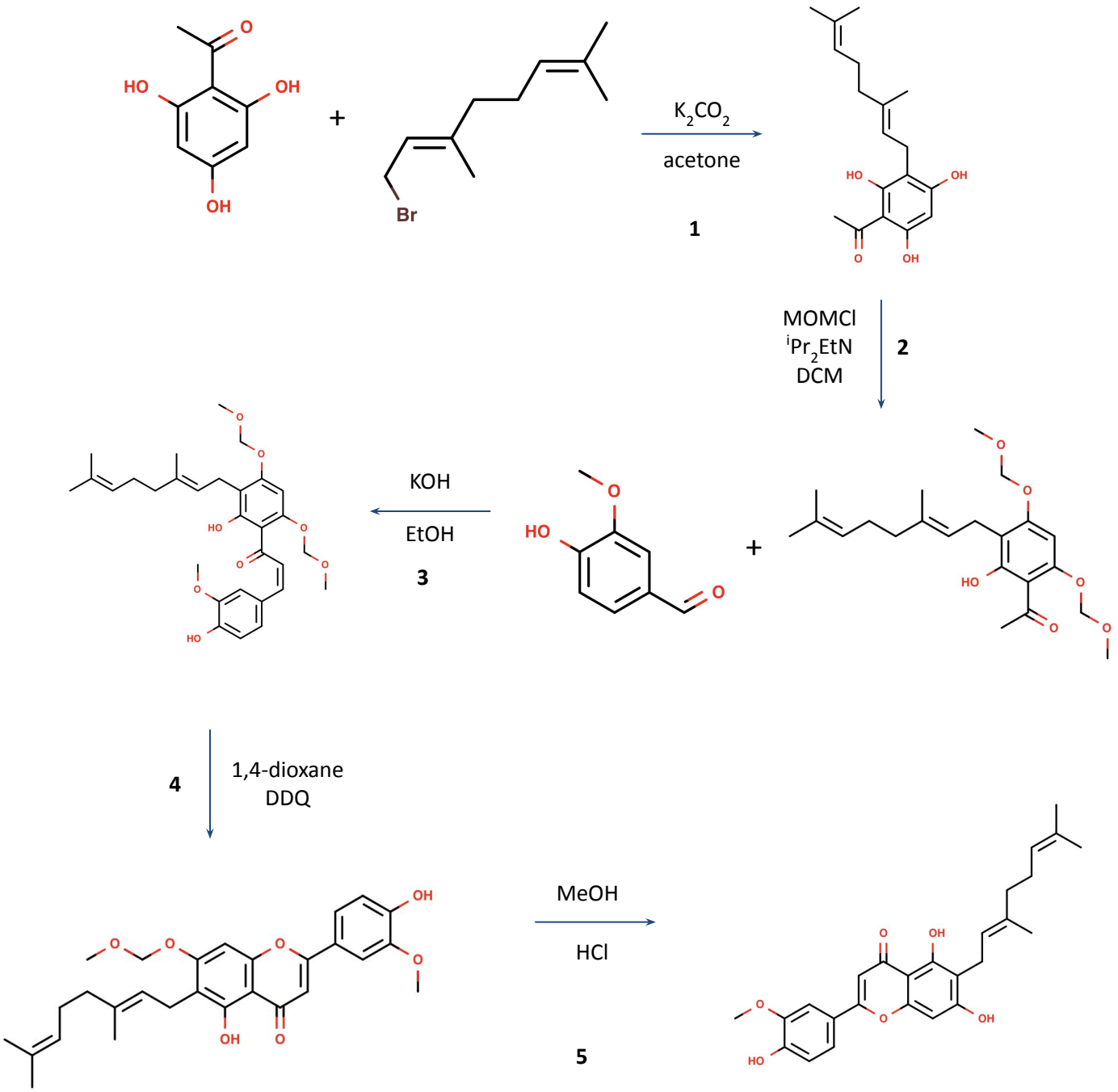
Solvent	Temperature	LogS	AI Choice
Ethyl Alcohol	298	0.244	Yes
Methyl Alcohol	298	0.300	Yes
Dichloromethane	298	0.456	Yes
n-hexane	298	-4.538	No
Ethyl Acetate	298	0.631	Partially
Trichloromethane	298	0.058	Partially
Ethyl Ether	298	-0.769	No
H20	298	-6.456	No
Dimethylformamide	298	2.210	Yes
DMSO	298	1.988	Yes

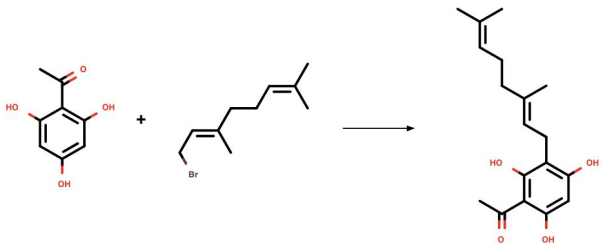
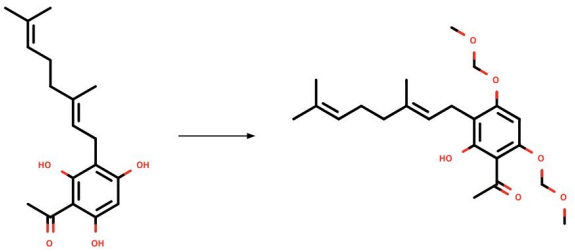
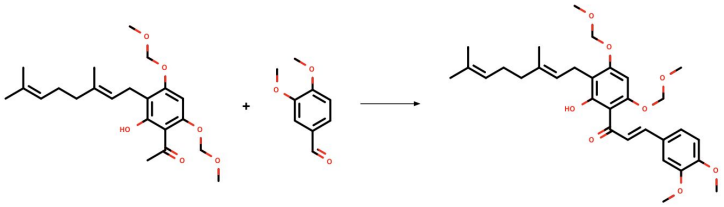
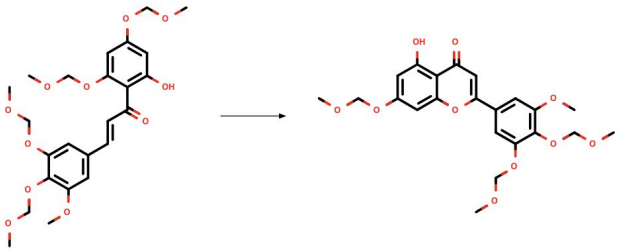
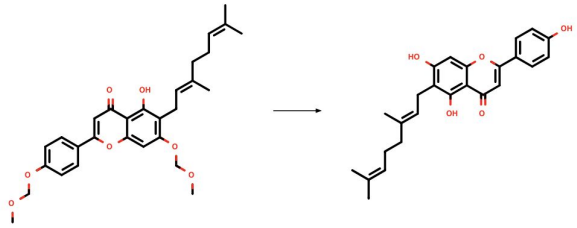
Solvate Prediction

Chemical	Solvent	Probability	AI Choice
Cannaflavin A	Water	0.9647	Yes
Cannaflavin A	Ethyl Alcohol	0.7124	Yes
Cannaflavin A	Methyl alcohol	0.9616	Yes
Cannaflavin A	Dichloromethane	1.0000	Yes
Cannaflavin A	n-Hexane	0.0782	No
Cannaflavin A	Ethyl acetate	0.9530	Yes
Cannaflavin A	Trichloromethane	1.0000	Yes
Cannaflavin A	Ethyl ether	0.7905	Yes
Cannaflavin A	Dimethylformamide	0.9827	Yes
Cannaflavin A	DMSO	0.9851	Yes
Cannaflavin A	Oxolane	0.9743	Yes

Polymorphism Predictions (Coming Soon)

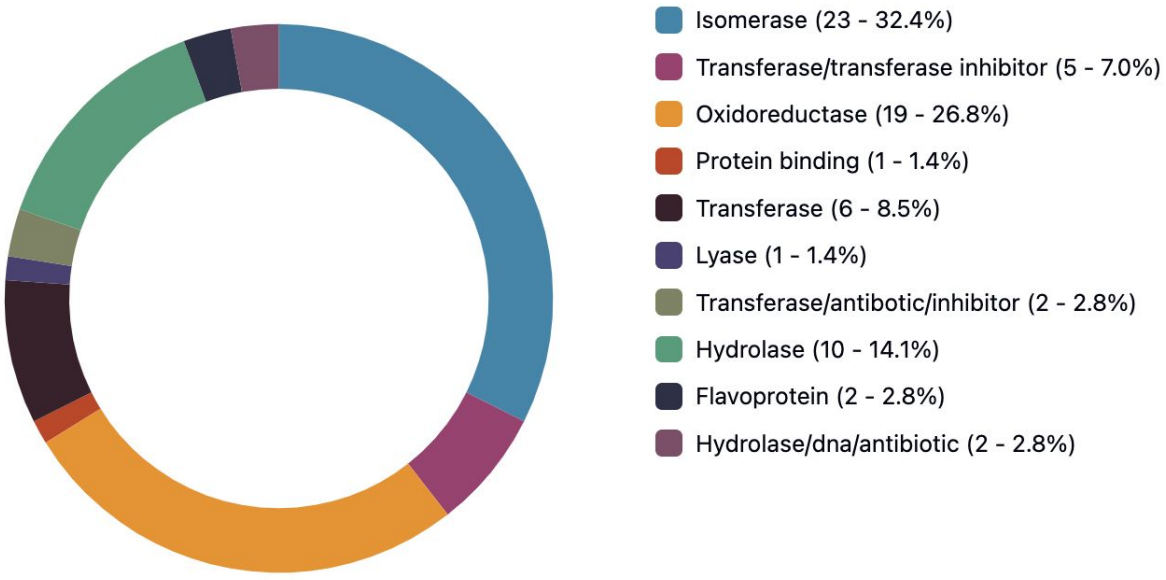
Green Retrosynthesis



Step	Reference Reaction	DOI
1		Sun, Qiu, et al. “Synthesis of Natural-like Acylphloroglucinols with Anti-Proliferative, Anti-Oxidative and Tube-Formation Inhibitory Activity.” European Journal of Medicinal Chemistry, vol. 85, Oct. 2014, pp. 621–28
2		Jung, Doo Hwan, et al. “New Synthetic Routes to Biologically Interesting Geranylated Flavanones and Geranylated Chalcones: First Total Synthesis of (±)-Prostratol F, Xanthoangelol, and (±)-Lespeol.” Helvetica Chimica Acta, vol. 93, no. 4, Apr. 2010, pp. 635–47.
3		Jung, Doo Hwan, et al. “New Synthetic Routes to Biologically Interesting Geranylated Flavanones and Geranylated Chalcones: First Total Synthesis of (±)-Prostratol F, Xanthoangelol, and (±)-Lespeol.” Helvetica Chimica Acta, vol. 93, no. 4, Apr. 2010, pp. 635–47.
4		Guz, Nathan R., and Frank R. Stermitz. “Synthesis and Structures of Regioisomeric Hydnocarpin-Type Flavonolignans.” Journal of Natural Products, vol. 63, no. 8, Aug. 2000, pp. 1140–45.
5		Heterocycles; vol. 32; 3; (1991); p. 499 - 510

Molecular Dynamic Analysis: 2D NMR Spectra & Dose Response Curves

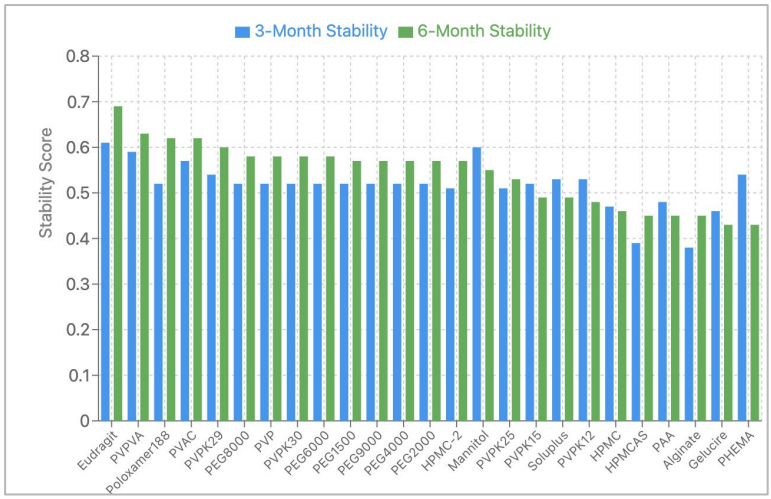
Chemical Disease Pathway

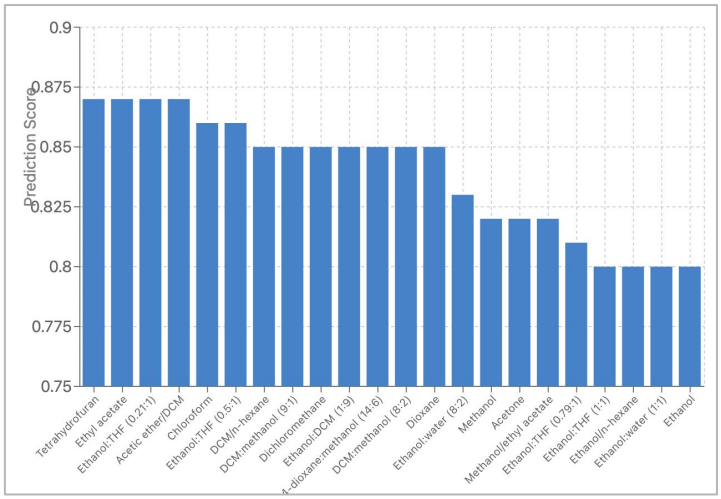


Target Distribution of Protein Families

Major Target Identified	PDB ID	Physiological Effects	Risks	Drug Before	Adverse Effects
PIM1	4XH6	Anti-inflammatory, Diabetes Mellitus, Obesity	Yes	Thioridazine	Hospitalization (initial or prolonged):24 Death: 22 Life-Threatening condition:6 Disability:4
RSK2	4GUE	Modulate cell proliferation, transformation, Cell Cycle transition	Yes	N/A	N/A

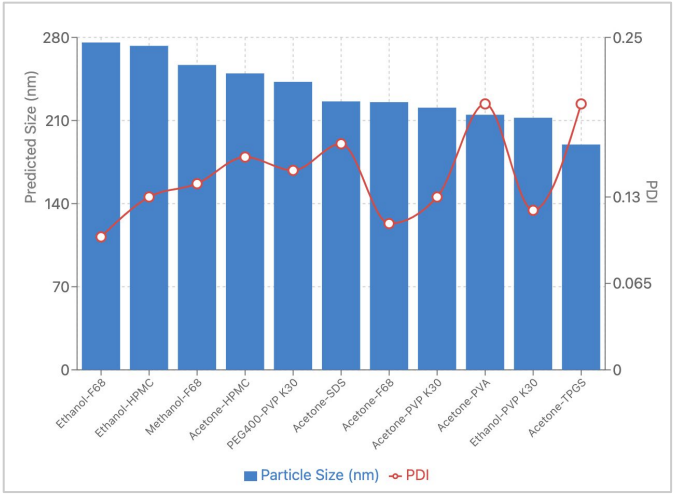
Formulation Profile



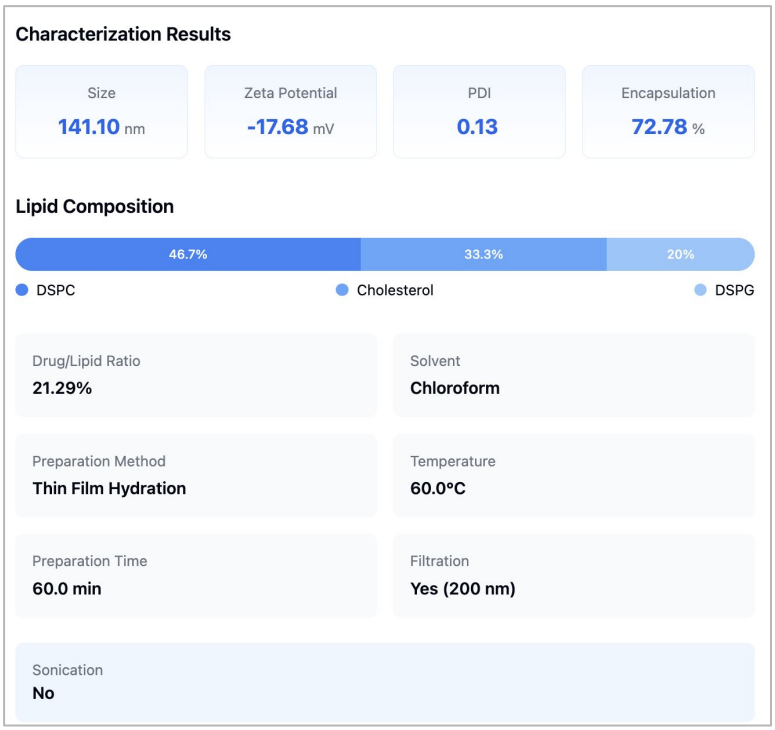


Solid Dispersions Stability
Technique: 1-Hot Melt Extrusion
Storage Temperature: 25.0°C
Preparation Temperature: 60.0°C
Relative Humidity: 75.0%

Phospholipid Complex Combination
Reaction Temperature: 50.0°C
Drug Phospholipid Ratio: 0.50
Reaction Time: 2.0h

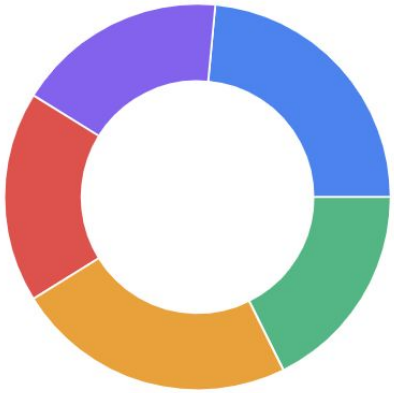


Nanosize Particle Predictions
Method: Anti-solvent
Concentration S1: 0.5
Volume Ratio: 0.1
Volume of Water: 2
Ultrasonication Time: 1.5
Stirring Speed: 1000
Ultrasonication Power: 300
Concentration API: 10



Formulation Risks

Excipient Hazard Flags



- **Alkaline excipients**
  Bentonite, Calcium Carbonate, Magnesium Oxide, Sodium Bicarbonate
- **Metal ion impurities**
  Calcium Alginate, Calcium Phosphate, Zinc Stearate
- **Oxidizing excipients**
  Acacia, Attapulgite, Calcium Oxide
- **Aldehyde impurities**
  HPMC, Lactose, PEG, Starch
- **Peroxide impurities**
  Lanolin, PVP, PVPP

The excipient risk analysis identifies five major risk categories that require careful consideration in formulation. The risk profile includes potential interactions with alkaline excipients (such as calcium carbonate and sodium bicarbonate), metal ion-containing excipients (like calcium alginate and zinc stearate), and oxidizing excipients (including acacia and calcium oxide). Additional concerns arise from excipients containing aldehyde impurities (such as HPMC, PEG, and starch) and peroxide impurities (found in materials like PVP and lanolin). These chemical interactions could affect drug stability and efficacy, necessitating careful excipient selection during formulation development.

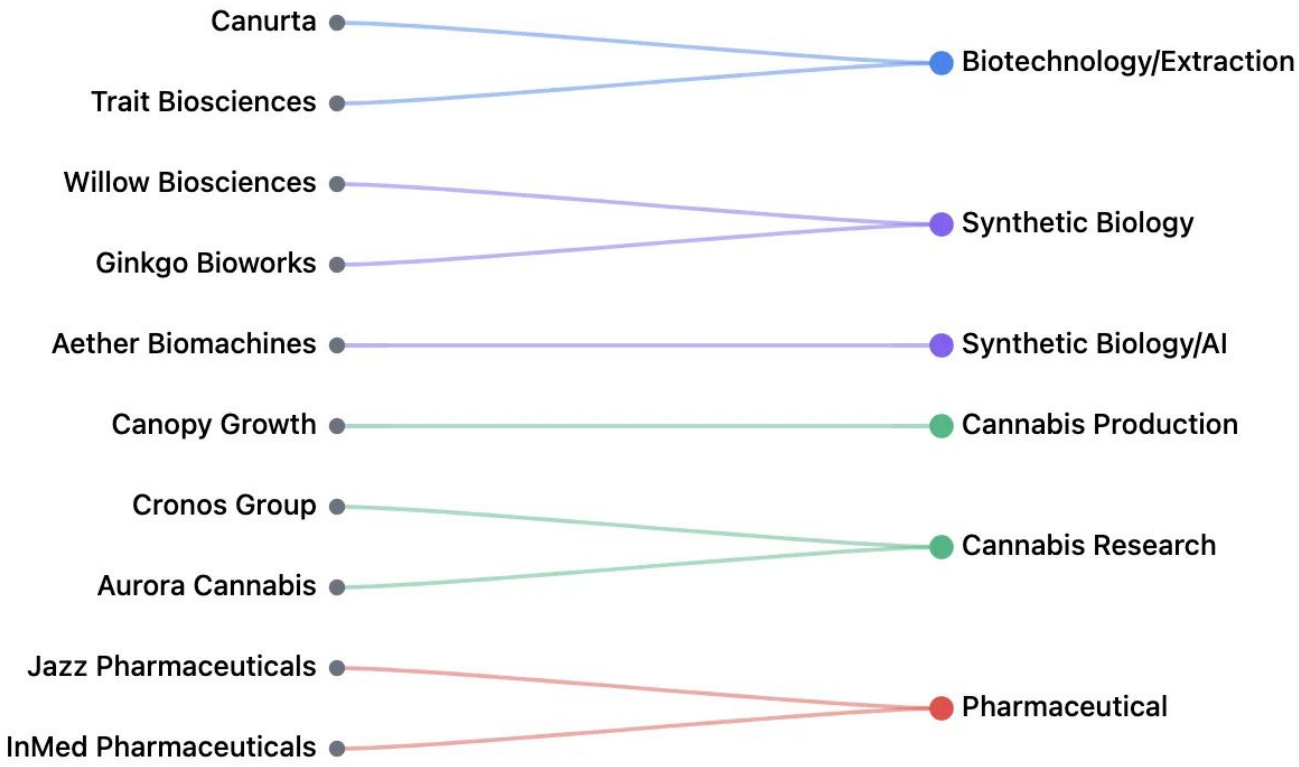
Toxicology Endpoints

Pulmonary embolism, pulmonary hypertensio	No
Drug-induced rhabdomyolysis	No
Acute oral toxicity	Yes
Toxicity on avian species	No
Honey bee toxicity	No
Reproductive and development toxicity	No
Nongenotoxic carcinogenicity	No
Inhalation toxicity	No
Drug-induced ototoxicity	No
Endocrine disruption-estrogen receptor	No
Eye irritation	No
Chemical-induced hematotoxicity	No
Endocrine disruption-pregnane X receptor	No
Mitochondrial toxicity	No
Bioconcentration	No
Chemical aquatic toxicity: Daphnia magna	Yes
Nephrotoxicity	Yes
Asthma-KRFP	No
Endocrine disruption-androgen receptor	No
Endocrine disruption	No
Drug-induced neurotoxicity	No
Drug-induced autoimmune diseases	No
Mitochondrial Toxicity	No
Skin sensitization	Yes
hERG inhibition	Yes
Pulmonary fibrosis-KRFP	No
Hepatotoxicity	Yes
Respiratory infection-KRFP	No
Pneumonia-KRFP	No
Chemical aquatic toxicity: Fathead minnow	No
Idiosyncratic adverse drug reaction	Yes
Bronchospasm-KRFP	Yes
Chemical aquatic toxicity: Tetrahymena pyrifo	Yes
Pulmonary edema-KRFP	No
Bronchitis-KRFP	Yes
Mutagenicity	Yes

The toxicological assessment reveals 11 positive endpoints out of 36 total endpoints tested. Key concerns include aquatic toxicity (affecting Daphnia magna and Tetrahymena), cardiac safety (hERG inhibition), and organ-specific toxicity (hepatotoxicity and nephrotoxicity). The compound also shows potential for acute oral toxicity, skin sensitization, and mutagenicity. Several respiratory-related effects are indicated, including bronchitis and bronchospasm. However, the compound shows no significant risks for many critical endpoints including reproductive toxicity, endocrine disruption, neurotoxicity, or carcinogenicity. The majority of KRFP (Knowledge-based Respiratory Failure Prediction) endpoints are negative.

Product Market

In the pursuit of Cannflavin A development, each industry sector brings unique approaches. Canurta leads specialized extraction with proprietary methods specifically for cannflavins, while Trait Biosciences focuses on water-soluble cannabinoid technology. In synthetic biology, Willow Biosciences and Ginkgo Bioworks are developing biosynthetic production methods for rare cannabinoids including Cannflavin A. Aether Biomachines applies AI to optimize biosynthesis processes. Traditional cannabis companies like Canopy Growth and Cronos Group incorporate Cannflavin A research into broader cannabinoid programs, while pharmaceutical companies Jazz and InMed explore medical applications of cannabis-derived compounds including flavonoids.



Customer Journals (Coming Soon)

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