In silico inquest reveals the efficacy of Cannabis in the treatment of Post-Covid-19 related neurodegeneration

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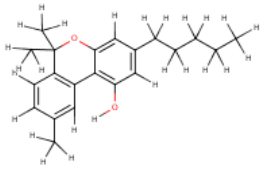
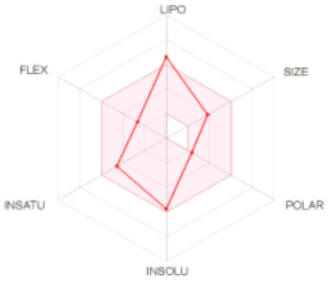
Physiochemical properties of CBD



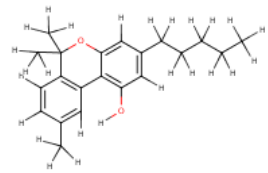


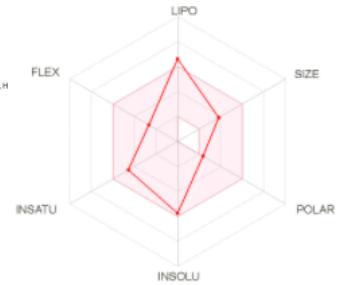
SMILES CCCCCc1cc(O)c2c(c1)OC(c1c2cc(C)cc1)(C)C

Physicochemical Properties	
Formula	C21H26O2
Molecular weight	310.43 g/mol
Num. heavy atoms	23
Num. arom. heavy atoms	12
Fraction Csp3	0.43
Num. rotatable bonds	4
Num. H-bond acceptors	2
Num. H-bond donors	1
Molar Refractivity	97.10
TPSA	29.46 Å²
Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.94
Log $P_{o/w}$ (XLOGP3)	6.11
Log $P_{o/w}$ (WLOGP)	5.62
Log $P_{o/w}$ (MLOGP)	4.23
Log $P_{o/w}$ (SILICOS-IT)	6.15
Consensus Log $P_{o/w}$	5.21

Water Solubility	
Log *S* (ESOL)	-5.74
Solubility	5.70e-04 mg/ml ; 1.84e-06 mol/l
Class	Moderately soluble
Log *S* (Ali)	-6.51
Solubility	9.59e-05 mg/ml ; 3.09e-07 mol/l
Class	Poorly soluble
Log *S* (SILICOS-IT)	-7.49
Solubility	1.00e-05 mg/ml ; 3.22e-08 mol/l
Class	Poorly soluble
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	Yes
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-3.86 cm/s
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	No; 1 violation: WLOGP>5.6
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: XLOGP3>5
Bioavailability Score	0.55
Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: XLOGP3>3.5
Synthetic accessibility	3.39

Physiochemical properties of CVN





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