

Drug-like properties of phytocannabinoids

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Phytocannabinoids could have therapeutic potential in a variety of pathological conditions regulated by endocannabinoid system. Hence, *in silico* analysis serves as powerful tool for the optimization of new therapeutic agents that target endocannabinoid system related diseases.

molinspiration
cheminformatics

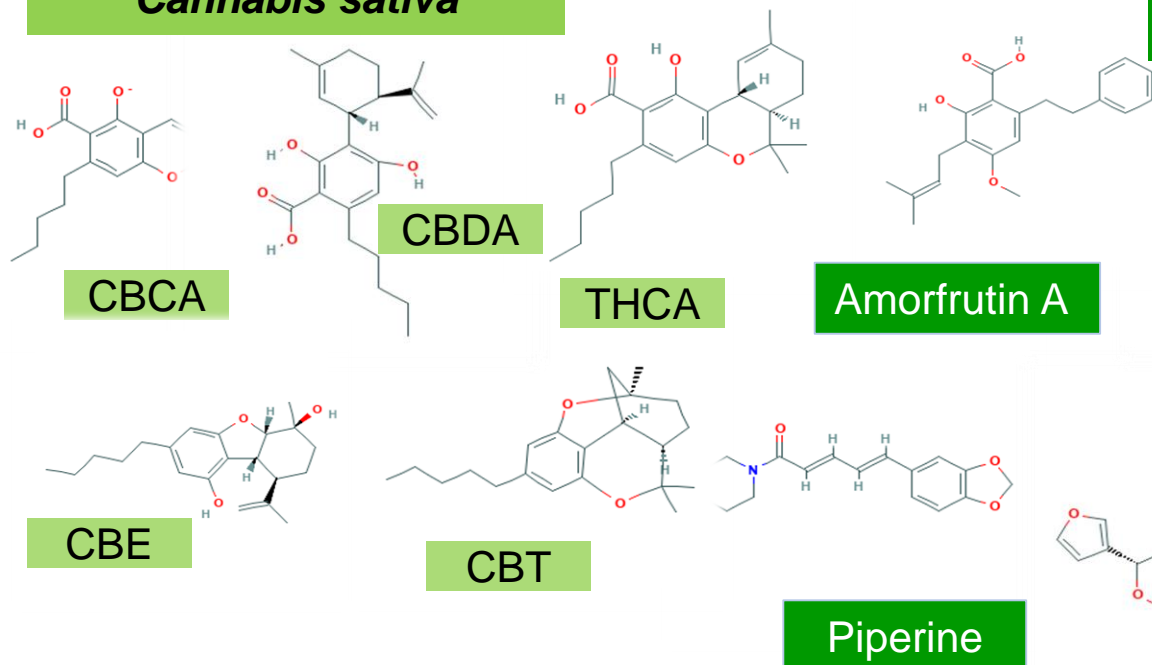


SwissADME

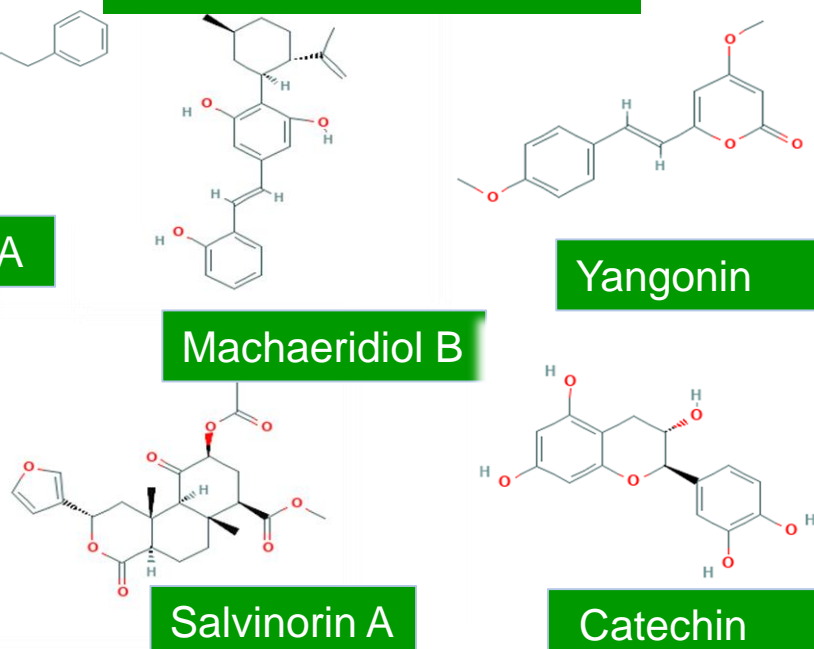


Phytocannabinoids

Cannabis sativa



Other natural resources



Group of compounds	GPCR	BBB	HIA	Caco-2
Endocannabinoids	0.06-0.35	0.75-0.91	0.88-0.99	0.50-0.54
Phytocannabinoids from <i>Cannabis sativa</i>	0.22-0.64	0.59-0.99	0.73-1	0.54-0.77
Compounds having similar structure to phytocannabinoids from <i>Cannabis sativa</i>	0.05-0.55	0.5-0.95	0.79-1	0.62-0.79
Alkaloids	-0.53-0.28	0.83-1	0.69-1	0.5-0.90
Terpenes	-0.34-0.50	0.77-0.98	0.97-1	0.54-0.89
Polyphenols	-0.23-0.41	0.52-0.91	0.59-1	0.71-0.95
Derivatives of fatty acids	-0.02-0.24	0.51-0.97	0.99-1	0.53-0.75

Molecular descriptors such as molecular weight (Mw), number of rotatable bonds, hydrogen bond acceptors and hydrogen bond donors (NHBA and NHBD, respectively), together with polar surface area (PSA), lipophilicity (MlogP) and solubility (logS) were calculated online for 80 compounds (endocannabinoids, phytocannabinoids from *Cannabis sativa* and phytocannabinoids from other natural resources) using Molinspiration and SwissADME programs. The human intestinal absorption and the permeability through Caco-2 cells were predicted by admetSAR tool. The enzyme inhibitory potential and the binding affinity to G-protein coupled receptors and nuclear receptors were calculated by Molinspiration program.

A more than half of the analysed compounds were in agreement with the requirements of Lipinski's and Veber's rules and would theoretically have appropriate oral bioavailability. In terms of drug-likeness, the analysed compounds could contribute to the discovery and optimization of suggesting drug candidates for the treatment of various pathological conditions.

92% of analyzed compounds had
M<500

71%
MlogP<4,15

95%
PSA<140

94%
nOHNH<5
nON<10

82%
nrotb ≤10

46% of analysed compounds met requirements set by Lipinski and Veber