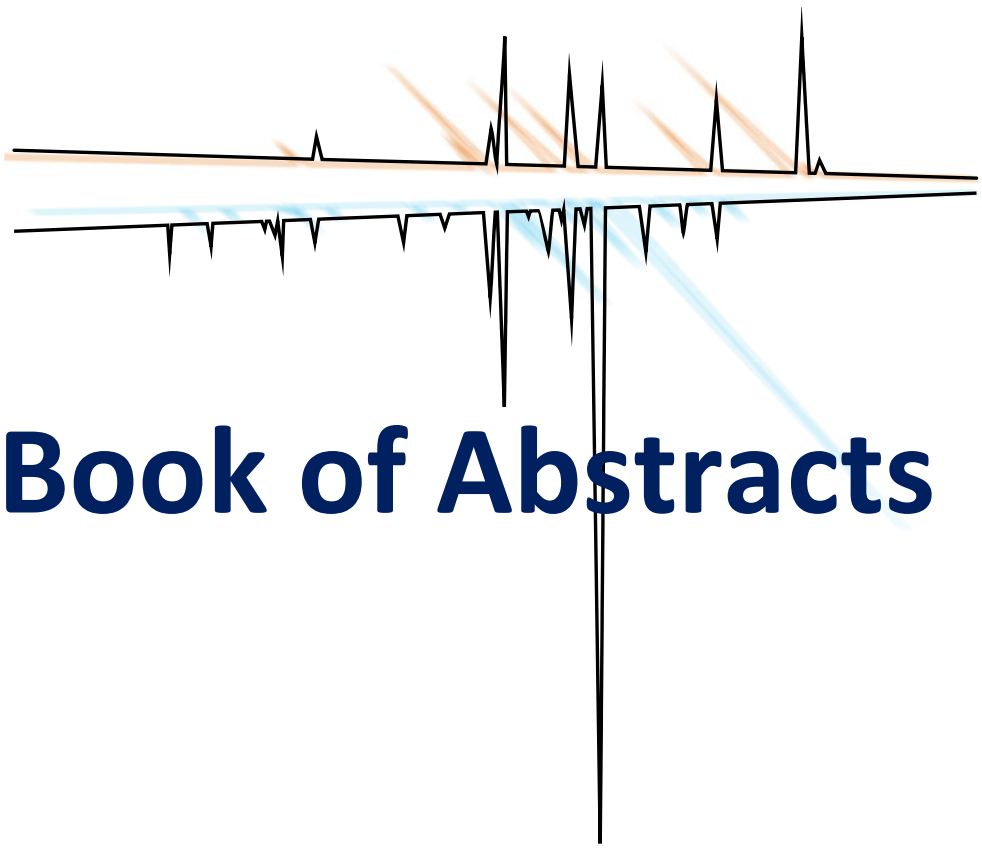
10th IAPC Meeting

Tenth World Conference on Physico-Chemical Methods in Drug Discovery & Sixth World Conference on ADMET and DMPK



Book of Abstracts

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Tenth World Conference on Physico-Chemical Methods in Drug Discovery
&
Sixth World Conference on ADMET and DMPK
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~~Withdrawn~~

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Computational study of interactions of *Cannabis Sativa* constituents with potential epigenetic targets involved in processes of multiple sclerosis

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Multiple sclerosis (MS) is a chronic inflammatory demyelinating and neurodegenerative disease, which treatment requires better understanding of underlying pathological processes. Epigenetic alterations as to some extent reversible processes might serve as another target for the therapy of MS for the aim of reprogramming inherited, environmentally initiated or by developing processes of MS influenced genotype and fenotype.
Cannabis sativa (CS) has been experimentally proven for positive outputs in treatment of MS, not just in elevating symptoms, but stopping the progress of disease. However, incidences of healing might focus further attention of wider impact of numerous constituents of CS that might play various roles in whole processes of possible healing, including epigenetic modulation. There are the proofs however that epigenetic changes are involved at certain stages of MS.
In this work, the potential of CS for treatment of altered epigenetic mechanisms involved in MS was investigated using network pharmacology methods. Constituents of CS were collected from literature, classified in few classes: cannabinoids, terpenoids, flavonoids, stilbenoids and alkaloids. Epigenetic targets (37) were chosen as overlap of predicted epigenetic targets for CS constituents by SwissTargetPrediction and EpigeneticTargetProfiler, as well as epigenetic targets involved in MS obtained from GeneCArds and DisGeNet data bases. The relevance of chosen targets is supported in literature, as asscosiated with various processes of MS.
Network of CS constituents and chosen targets was mapped and analyzed by Cytoscape 3.9.1. Among the network consisted of 71 nodes and 266 edges, 266 interactions between CS constituents and epigenetic targets were indicated. The degree analysis of the obtained netwok was performed from the aspect of particular compound for possible targets and particular target for possible compounds interactions. Predictions of compunds and targets interactions are based on molecular similarity, therefore it remains to be further explored are those possible interactions associated with agonistic or antagonistic effects of the compounds. Promising results regarding possible interactions of CS constituents on epigenetic level of MS processes might be helpful for consideration of the therapy by this medical plant at various stages of MS development, taking into account other possible interactions with targets out of epigenetic landscape, associated with MS as well.