marine drugs

MDPI

Supplementary materials

Marine drugs

Special issue - Marine Products with Anti-allergic and Anti-inflammatory Activities

(–)-Loliolide isolated from Sargassum horneri abate UVB-induced oxidative damage in human dermal fibroblasts and subside ECM degradation

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HTT attenuated intracellular ROS level in UVB exposed HDFs

Intracellular ROS levels of HDFs were analyzed by fluorescence microscopy and flow cytometry. Per Figure S1A and S1B, UVB exposure caused a significant increase in intracellular ROS levels indicated by increased green fluorescence intensity compared to the control. HTT treated HDFs indicated a dose dependent reduction of the fluorescence intensity suggesting its ROS inhibitory effects.

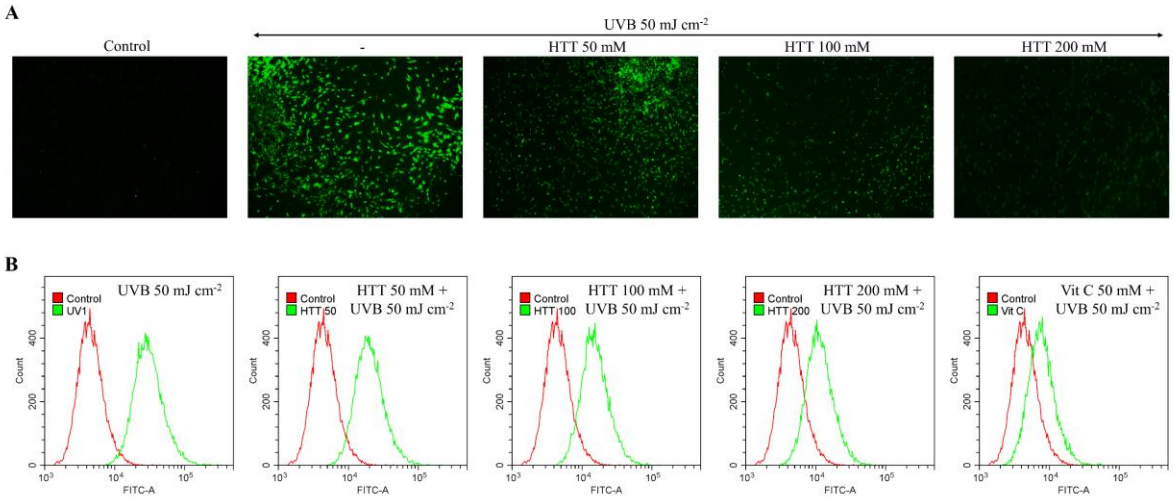

Figure S1. Effects of HTT in reducing UVB-induced intracellular ROS levels. Evaluation of ROS levels by (A) fluorescence microscopy and (B) flow cytometry. Intracellular ROS level was measured 2h after the stimulation. The cells were stained with 2′ 7′-dichlorodihydrofluorescein diacetate (DCF-DA). Results represent the mean ± SD (error bars) of three independent experimental trials (n=3). Bars with different letters are significantly different at $P < 0.05$.

Predicting skin permeability of HTT

The effectivity of a drug candidate depends on numerous pharmacokinetic parameters including the stability and bioavailability of the drug at the target site, for a sufficient duration. Herein the skin permeability of HTT should be substantial to employ it as a UVB protective substance. The skin permeability of an exposed drug is generally evaluated by determining the skin permeation coefficient (Kp) of the drug in the stratum corneum. However, numerous constraints limit the experimental evaluation of Kp value. The analysis utilizes the Kp calculation available from SwissADME free web tool (http://www.swissadme.ch/index.php) [1], initially developed based on QSAR model developed by Potts and Guy [2]. The skin permeability of a drug is mainly determined by molecular size and lipophilicity. HTT indicated a Log Kp value of -6.79 cm/s indicating that it is desirable to employ in topical applications. According to the model by Potts and Guy, the lowest estimated permeability was reported for clindamycin (Log Kp = -9.6) while the highest predicted permeability values are reported for lipophilic compounds such as bexarotene (Log Kp = -4.5), tazarotene (Log Kp = -4.7) and adapalene (Log Kp = -5.3) [2].

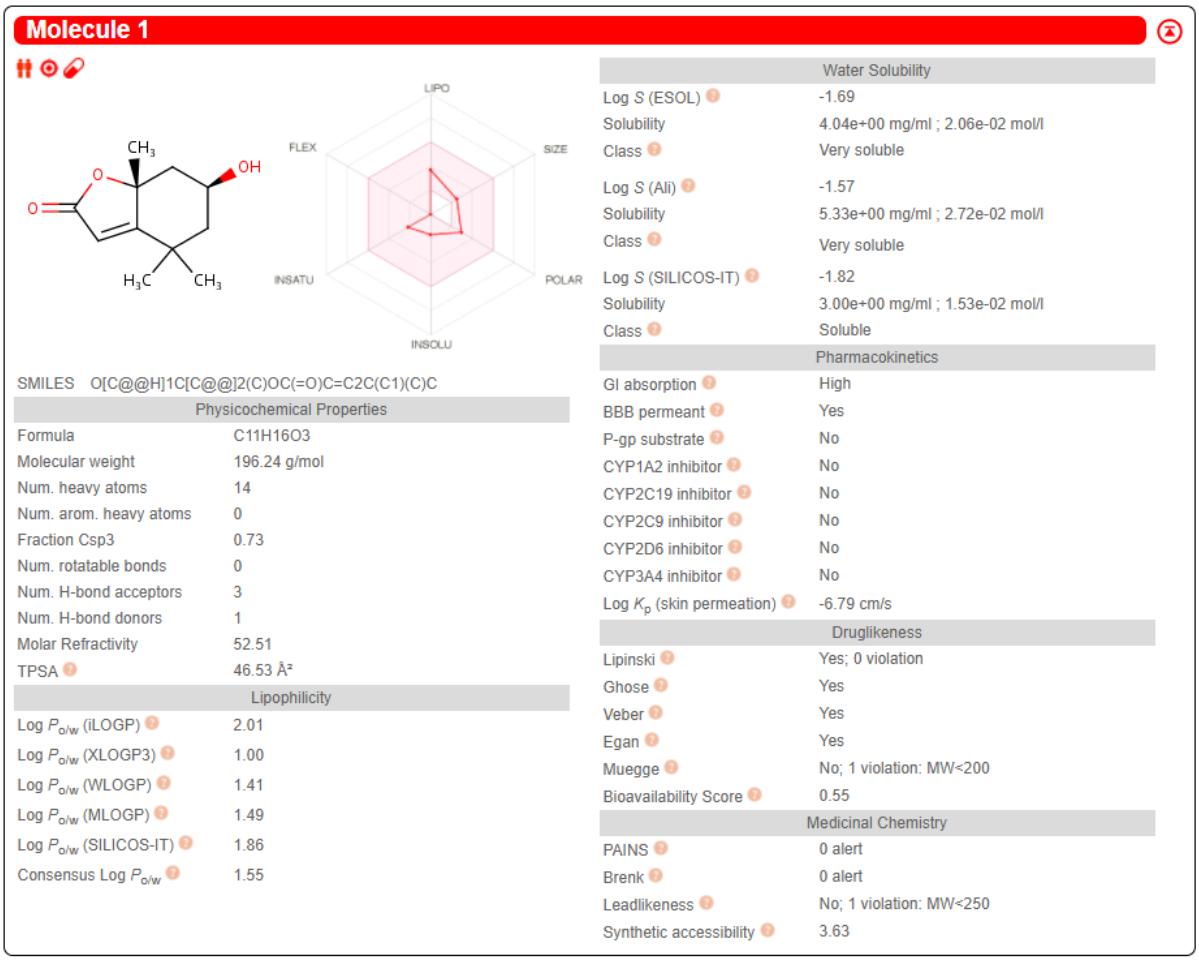

Figure S2. Predicted physicochemical descriptors, ADME parameters and pharmacokinetic properties of HTT to act as a drug. The calculation was carried out by submitting the SMILES specifications of HTT to SwissADME free web tool (http://www.swissadme.ch/index.php).

References

1. Hay, M.; Thomas, D. W.; Craighead, J. L.; Economides, C.; Rosenthal, J., Clinical development success rates for investigational drugs. *Nature Biotechnol.* **2014,** 32.
2. Potts, R. O.; Guy, R. H., Predicting skin permeability. *Pharm. Res.* **1992,** 9, (5), 663-669.