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## Hepatoprotection of Sesquiterpenoids: A Quantitative Structure-Activity Relationship (QSAR) Approach

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### Abstract

The relative hepatoprotection effect of fifteen sesquiterpenoids, commonly found in plants and plant-derived foods and beverages was assessed. Endogenous lipid peroxidation (assay A) and induced lipid peroxidation (assay B) were evaluated in liver homogenates from Wistar rats by the thiobarbituric acid reactive species test. Sesquiterpenoids with different chemical structures were tested: trans,trans-farnesol, cis-nerolidol, (-)- $\alpha$ -bisabolol, trans- $\beta$ -farnesene, germacrene D,  $\alpha$ -humulene,  $\beta$ -caryophyllene,  $\alpha$ -bisabolol, (+)-valencene, guaiazulene, (-)- $\alpha$ -cedrene, (+)-aromadendrene, (-)- $\alpha$ -neocladol, (+)-cyclosativene. Ascorbic acid was used as a positive antioxidant control. With ascorbic acid, all the sesquiterpenoids under study (1mM) were effective in reducing the malondialdehyde levels in both endogenous and induced lipid peroxidation up to 35% and 70%, respectively.

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models developed, relating the hepatoprotection activity with molecular properties, showed good fit (Radj(2) 0.819 and 0.972 for the assays A and B, respectively) with good prediction power ( $Q(2) > 0.950$  and  $SDEP < 2\%$ , for both models A and B). A network of effects associated with structural and chemical features of sesquiterpenoids such as shape, branching, symmetry, and presence of electronegative fragments, can modulate the hepatoprotective activity observed for these compounds.

**Keywords:** Hepatoprotection; Lipid peroxidation; Quantitative structure–activity relationship; Rat hepatocytes; Sesquiterpenoids; TBARS.

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## Assessment of the Antioxidant and Antiproliferative Effects of Sesquiterpenic Compounds in in Vitro Caco-2 Cell Models

J Vinholes et al. *Food Chem* 156, 204-11. 2014. PMID 24629959.

In this study, the antiradical and antiproliferative effects of the sesquiterpenic compounds trans, trans-farnesol, cis-nerolidol,  $\alpha$ -humulene and guaiazulene, commonly fo ...

## Cytotoxic and Antioxidative Sesquiterpenoids From *Heterotheca Inuloides*

I Kubo et al. *Planta Med* 62 (5), 427-30. Oct 1996. PMID 8923808.

Four sesquiterpenoids, beta-caryophyllene, beta-caryophyllene 4,5 alpha-oxide, 7-hydroxy-3,4-dihydrocadalin, and 7-hydroxycadalin, isolated from the dried flower of Heter ...

## Assessment of Antioxidant Activity of Eugenol in Vitro and in Vivo

E Nagababu et al. *Methods Mol Biol* 610, 165-80. 2010. PMID 20013178.

Reactive oxygen species are implicated in many human diseases and aging process. Much of the evidence is based on experimental data indicating increasing rates of lipid p ...

## [Reviews on Natural Monocyclic Sesquiterpenoids and Their Bioactivities]

J Fu et al. *Zhongguo Zhong Yao Za Zhi* 44 (17), 3672-3683. Sep 2019. PMID 31602939. - *Review*

Sesquiterpenes are a class of terpenoids composed of three isoprene units( 15 carbons). Sesquiterpenoids possess a variety of different structures,including acyclic sesqu ...

## [Phytochemical and Pharmacological Progress on Humulane-Type Sesquiterpenoids]

SG Jiao et al. *Zhongguo Zhong Yao Za Zhi* 43 (22), 4380-4390. Nov 2018. PMID 30593228. - *Review*

Humulane-type sesquiterpenoids, widely distributed in plants and microbes, include three types:  $\alpha$ -humulene,  $\beta$ -humulene, and  $\gamma$ -humulene. Up to now, 98 humulane-type sesqui ...

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R Perestrelo et al. *Foods* 8 (12). 2019. PMID 31805724.

Terpenoids, including monoterpenoids (C<sub>10</sub>), norisoprenoids (C<sub>13</sub>), and sesquiterpenoids (C<sub>15</sub>), constitute a large group of plant-derived n ...

## PHYTOCHEMICAL, ELEMENTAL AND BIOTECHNOLOGICAL STUDY OF *CRYPTOCARYA LATIFOLIA*

MF Hamza et al. *Afr J Tradit Complement Altern Med* 13 (4), 74-80. 2016. PMID 28852722.

This study validates the ethno-medicinal use of the plant and supports the replacement of bark and roots by leaves and fruits for the management and conservation of this ...

## Pharmacological Potential of Phylogenetically Diverse Actinobacteria Isolated From Deep-Sea Coral Ecosystems of the Submarine Avilés Canyon in the Cantabrian Sea

A Sarmiento-Vizcaíno et al. *Microb Ecol* 73 (2), 338-352. Feb 2017. PMID 27614749.

Marine Actinobacteria are emerging as an unexplored source for natural product discovery. Eighty-seven deep-sea coral reef invertebrates were collected during an oceanogr ...

## Nerolidol: A Sesquiterpene Alcohol With Multi-Faceted Pharmacological and Biological Activities

WK Chan et al. *Molecules* 21 (5). 2016. PMID 27136520. - *Review*

Nerolidol (3,7,11-trimethyl-1,6,10-dodecatrien-3-ol) is a naturally occurring sesquiterpene alcohol that is present in various plants with a floral odor. It is synthesized ...

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### Previous result

[In vivo genotoxicity assessment of nerolidol.](#)

[Pículo F, et al. J Appl Toxicol 2011.](#)

The objective of this study was to evaluate the ability of a single **nerolidol** treatment to induce DNA damage in peripheral blood and **liver** cells of mice and micronuclei in polychromatic erythrocytes of bone marrow cells of the same animals. ...The data obtained support the view that **nerolidol** induces clastogenicity and very weak genotoxicity in the mouse cells tested....

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[Phytomedical assessment of two Cymbopogon species found in Nkonkobe Municipality: toxicological effect on human Chang \*\*liver\*\* cell line.](#)

[Omoruyi BE and Muchenje V. BMC Complement Altern Med 2017.](#)

Total oil percentage of *C. plurinodis* was 81.47% and the main components were characterized as 3-Cyclohexane-1-ol (13.58%), **Nerolidol** (13.6%) and 2-Carene (12.6%). ...CONCLUSION: Both plants extracts were toxic to human Chang **liver** cell lines....

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