

Design and synthesis of eugenol derivatives, as potent 15-lipoxygenase inhibitors

Sadeghian, H.^a, Seyedi, S.M.^a, Saberi, M.R.^b, Arghiani, Z.^a, Riazi, M.^a

^a Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, 91770-1436, Iran

^b School of Pharmacy, Pharmaceutical Research Center, Mashhad University of Medical Sciences, BuAli Square, Mashhad 9196773117, Iran

[View references \(5\)](#)

Abstract

A group of ϵ -allyl- γ -methoxyphenol (eugenol) esters were designed, synthesized, and evaluated as potential inhibitors of soybean 15-lipoxygenase (SLO). Compounds ϵ c, ϵ d, ϵ f, ϵ p, and ϵ q showed the best IC₅₀ in SLO inhibition (IC₅₀ = 1.5, 2.3, 2.1, 2.2, and 0.15 μ M, respectively). All compounds were docked into SLO active site and showed that allyl group of compounds is oriented toward the iron atom in the active site of SLO. It is assumed that lipophilic interaction of ligand-enzyme would be in charge of inhibiting the enzyme activity. The selectivity of eugenol derivatives in inhibiting 15-HLOb was also compared with 15-HLOa by molecular modeling and multiple alignment techniques. © 2007 Elsevier Ltd. All rights reserved.

Reaxys Database Information

[View Compounds](#) [View Reactions](#)

Author keywords

15-HLOa; 15-HLOb; ϵ -Allyl- γ -methoxyphenol; Docking; Protein modeling; Soybean lipoxygenase

Indexed Keywords

EMTREE drug terms: 15 lipoxygenase inhibitor; ϵ allyl γ methoxyphenyl γ adamantanecarboxylate; ϵ allyl γ methoxyphenyl γ cyclohexanecarboxylate; ϵ allyl γ methoxyphenyl γ chlorobenzoate; ϵ allyl γ methoxyphenyl γ fluorobenzoate; ϵ allyl γ methoxyphenyl γ methylbenzoate; ϵ allyl γ methoxyphenyl γ pyridinecarboxylate; ϵ allyl γ methoxyphenyl γ chlorobenzoate; ϵ allyl γ methoxyphenyl γ fluorobenzoate; ϵ allyl γ methoxyphenyl γ methoxybenzoate; ϵ allyl γ methoxyphenyl ϵ chlorobenzoate; ϵ allyl γ methoxyphenyl ϵ fluorobenzoate; ϵ allyl γ methoxyphenyl ϵ methoxybenzoate; ϵ allyl γ methoxyphenyl ϵ methylbenzoate; ϵ allyl γ methoxyphenyl benzoate; ϵ allyl γ methoxyphenyl isonicotinate; ϵ allyl γ methoxyphenyl nicotinate; arachidonate 15 lipoxygenase; eugenol; iron; ligand; lipoxygenase inhibitor; unclassified drug

EMTREE medical terms: article; comparative study; drug design; drug screening; drug synthesis; enzyme activity; enzyme inhibition; IC₅₀; lipophilicity; molecular model

MeSH: Amino Acids; Arachidonate 15-Lipoxygenase; Combinatorial Chemistry Techniques; Crystallography, X-Ray; Drug Design; Eugenol; Lipoxygenase Inhibitors; Models, Molecular; Molecular Conformation; Molecular Structure; Quantitative Structure-Activity Relationship; Soybeans

Medline is the source for the MeSH terms of this document.

Species Index: Glycine max

Chemicals and CAS Registry Numbers: arachidonate 15 lipoxygenase, 82249-77-2; eugenol, 97-03-0; iron, 14093-02-8, 03808-86-9, 7439-89-6; Amino Acids; Arachidonate 15-Lipoxygenase, 1,13,11,33; Eugenol, 97-03-0; Lipoxygenase Inhibitors

ISSN: 0968-0896 CODEN: BMECES Source Type: Journal Original language: English