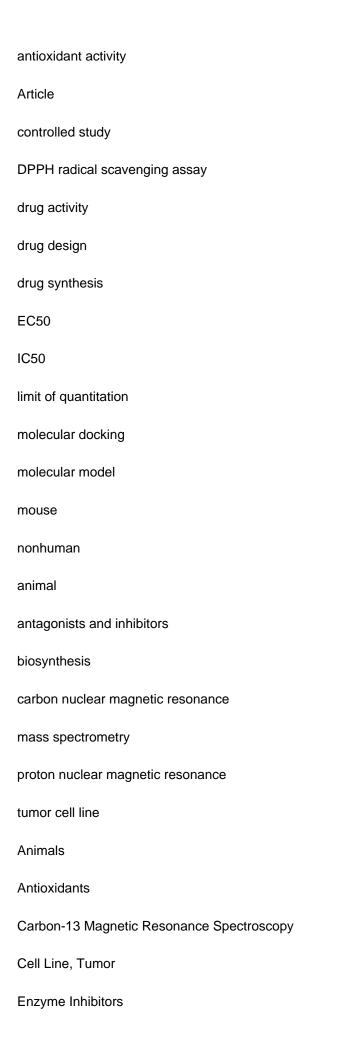
New insights into highly potent tyrosinase inhibitors based on 3-heteroarylcoumarins: Anti-melanogenesis and antioxidant activities, and computational molecular modeling studies

Pintus F.
Matos M.J.
Vilar S.
Hripcsak G.
Varela C.
Uriarte E.
Santana L.
Borges F.
Medda R.
Di Petrillo A.
Era B.
Fais A.
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Melanogenesis is a physiological pathway for the formation of melanin. Tyrosinase catalyzes the first step of this process and down-regulation of its activity is responsible for the inhibition of melanogenesis. The search for molecules capable of controlling hyperpigmentation is a trend topic in health and cosmetics. A series of heteroarylcoumarins have been synthesized and evaluated. Compounds 4 and 8 exhibited higher tyrosinase inhibitory activities (IC50= 0.15 and 0.38 ?M, respectively), than the reference compound, kojic acid (IC50= 17.9 ?M). Compound 4 acts as competitive, while compound 8 as uncompetitive inhibitor of mushroom tyrosinase. Furthermore, compounds 2 and 8 inhibited tyrosinase activity and melanin production in B16F10 cells. In addition, compounds 2?4 and 8 proved to have an interesting antioxidant profile in both ABTS and DPPH radicals scavenging assays. Docking experiments were carried out in order to study the interactions between these heteroarylcoumarins and mushroom tyrosinase. © 2017 Elsevier Ltd

3-Heteroarylcoumarins
B16F10 melanoma cells
Melanogenesis
Tyrosinase inhibitors
3 (4 bromothiophen 2 yl) 5,7 dihydroxycoumarin
3 (4 bromothiophen 2 yl) 6 methoxycoumarin
3 (4 bromothiophen 2 yl) 7 hydroxycoumarin
3 (4 bromothiophen 2 yl) 7,8 dihydroxycoumarin
3 (4 bromothiophen 2 yl) 8 hydroxycoumarin
3 heteroarylcoumarin derivative
5,7 dihydroxy 3 (thiophen 2 yl)coumarin
6 hydroxy 3 (thiophen 2 yl)coumarin
6 methoxy 3 (thiophen 2 yl)coumarin
7 hydroxy 3 (thiophen 2 yl)coumarin
antioxidant
coumarin derivative
kojic acid
trolox C
unclassified drug
antioxidant
enzyme inhibitor
melanin
monophenol monooxygenase
ABTS radical scavenging assay
animal cell
antimelanogenesis activity



Melanins
Mice
Models, Molecular
Molecular Docking Simulation
Monophenol Monooxygenase
Proton Magnetic Resonance Spectroscopy

Mass Spectrometry