Synthesis, biological evaluation, and molecular simulation of chalcones and aurones as selective MAO-B inhibitors

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A series of chalcones and aurones were synthesized and evaluated in vitro as monoamine oxidase inhibitors (MAOi). Our results show that aurones, which had not been previously reported as MAOi, are MAO-B inhibitors. Thus, both families inhibited selectively the B isoform of MAO in the micromolar range, offering novel scaffolds for the design of new and potent MAO inhibitors. The main structural requirements for their activity were characterized with the aid of 3D-QSAR and docking studies.

aurones

chalcones

molecular modeling

monoamine oxidase inhibitors

QSAR

1 (2 hydroxy 5 methoxyphenyl) 3 (2,4,5 trimethoxyphenyl)prop 2 en 1 one

1 (2 hydroxy 6 methoxyphenyl) 3 (2,4,5 trimethoxyphenyl)prop 2 en 1 one

2 (2,3 dimethoxybenzylidene) 4 methoxybenzofuran 3(2h) one

2 (2,3 dimethoxybenzylidene) 5 methoxybenzofuran 3(2h) one

2 (2,4,5 trimethoxybenzylidene) 4 methoxybenzofuran 3(2h) one

2 (2,4,5 trimethoxybenzylidene) 5 methoxybenzofuran 3(2h) one

2 (2,5 dimethoxybenzylidene) 4 methoxybenzofuran 3(2h) one

2 (2,5 dimethoxybenzylidene) 5 methoxybenzofuran 3(2h) one

2 (4 bromo 2,5 dimethoxybenzylidene) 4 methoxybenzofuran 3(2h) one

2 (4 bromo 2,5 dimethoxybenzylidene) 5 methoxybenzofuran 3(2h) one

3 (2,3 dimethoxyphenyl) 1 (2 hydroxy 5 methoxyphenyl)prop 2 en 1 one

3 (2,3 dimethoxyphenyl) 1 (2 hydroxy 6 methoxyphenyl)prop 2 en 1 one

3 (2,5 dimethoxyphenyl) 1 (2 hydroxy 5 methoxyphenyl)prop 2 en 1 one

3 (2,5 dimethoxyphenyl) 1 (2 hydroxy 6 methoxyphenyl)prop 2 en 1 one

3 (4 bromo 2,5 dimethoxyphenyl) 1 (2 hydroxy 5 methoxyphenyl)prop 2 en 1 one

3 (4 bromo 2,5 dimethoxyphenyl) 1 (2 hydroxy 6 methoxyphenyl)prop 2 en 1 one

amine oxidase (flavin containing) isoenzyme B

aurone derivative

chalcone derivative

monoamine oxidase B inhibitor

natural products and their synthetic derivatives

unclassified drug

amine oxidase (flavin containing)

aurone

benzofuran derivative

chalcone derivative

monoamine oxidase inhibitor

Article

biological activity

drug design

drug screening

drug synthesis

enzyme inhibition

human

IC50

in vitro study

molecular docking

molecular dynamics

molecular mechanics

molecular model

nonhuman

priority journal

quantitative structure activity relation

rat

chemistry

metabolism

synthesis

Benzofurans

Chalcones

Humans

Molecular Docking Simulation

Monoamine Oxidase

Monoamine Oxidase Inhibitors

Quantitative Structure-Activity Relationship