Synthesis, 5-hydroxytryptamine1A receptor affinity and docking studies of 3-[3-(4-aryl-1-piperazinyl)-propyl]-1H-indole derivatives

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A series of 3-[3-(4-aryl-1-piperazinyl)-propyl]-1H-indole derivatives (12a-h) was synthesized and evaluated for binding affinity at the human 5-hydroxytryptamine1A receptor (5-HT1AR) compounds (12b) and (12h) showed the highest 5-HT1A receptor affinity (IC 50-=15 nM). Molecular docking studies with all the compounds in a homology model of 5-HT1A showed that the main interaction anchoring the ligand in the receptor was a charge-reinforced bond between the protonated nitrogen atom (N-4) of the piperazine ring and Aspartate3.32.

Binding

Docking

Indolylalkylarylpiperazine

Synthesis

3 [3 (4 pyrimidin 2 yl 1 piperazinyl) propyl] 1h indol

3 [3 [4 (2 methoxyphenyl) 1 piperazinyl] propyl] 1h indol

aspartic acid

indole derivative

ligand

piperazine

serotonin 1A receptor

unclassified drug

indole derivative

piperazine derivative

serotonin 1A receptor

article

binding affinity

controlled study

drug synthesis

human

human cell

molecular docking

receptor affinity

binding site

chemistry

computer simulation

metabolism

protein tertiary structure

structure activity relation

synthesis

Aspartic Acid

Binding Sites

Computer Simulation

Humans

Indoles

Piperazines

Protein Structure, Tertiary

Receptor, Serotonin, 5-HT1A

Structure-Activity Relationship