

Srpsko hemijsko društvo



Serbian Chemical Society

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Srpskog hemijskog društva**

**KRATKI IZVODI
RADOVA
KNJIGA RADOVA**

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the Serbian Chemical Society**

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BH-U-3

Katinoni kao stimulatori 5-HT_{2A}R receptora: Definisane bioaktivne konformacije 3-D QSAR profila kao načina za razumevanje njihovog ponašanja kao zloupotrebljivanih droga i dizajn anti-katinona

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Katinoni su poznate zloupotrebjavane droge sa slabo poznatom farmakologijom. Farmakološki profil komercijalno dostupnih katinona ispitivan je na nivou 5-HT_{2A} receptora, molekulskim dokovanjem, pomoću AutoDock Vina, i 3-D QSAR modelima pomoću Open3DQSAR. Potom su 3-D QSAR modeli sumirani u univerzalni SAR model, korišćen za dizajn inovativnih anti-katinona, potencijalnih blokatora dejstva katinona čija je farmakologija procenjena na nivou receptora pomoću molekulskog dokovanja. Dobijena pravila za dizajn antikatinona pružaju mogućnost za dalju sintezu i biološku evaluaciju.

Cathinones as 5-HT_{2A}R stimulators: Definition of bioactive conformations and 3-D QSAR profiles as a pathway for understanding their behavior as abusing drugs and design of anti-cathinones

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Cathinones are known abusing drugs with pharmacology fairly known. Commercially available cathinones' pharmacodynamics profiles were elaborated on the 5-HT_{2A}R level with the aid of AutoDock Vina-based molecular docking and Open3DQSAR-based 3-D QSAR studies. Following, 3-D QSAR models were summarized in universal SAR models, further used to design innovative anti-cathinones, with the potential potency to block cathinones' action and pharmacology assessed using molecular docking. The obtained design rules provided the opportunity for further synthesis and biological evaluation.

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