

**VRE for regional Interdisciplinary
communities in Southeast Europe and
the Eastern Mediterranean**

**KOMPARACIJA RAČUNARSKOG MODELA
MOLEKULA SA EKSPERIMENTALNIM
REZULTATIMA**

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Prirodno-matematički fakultet
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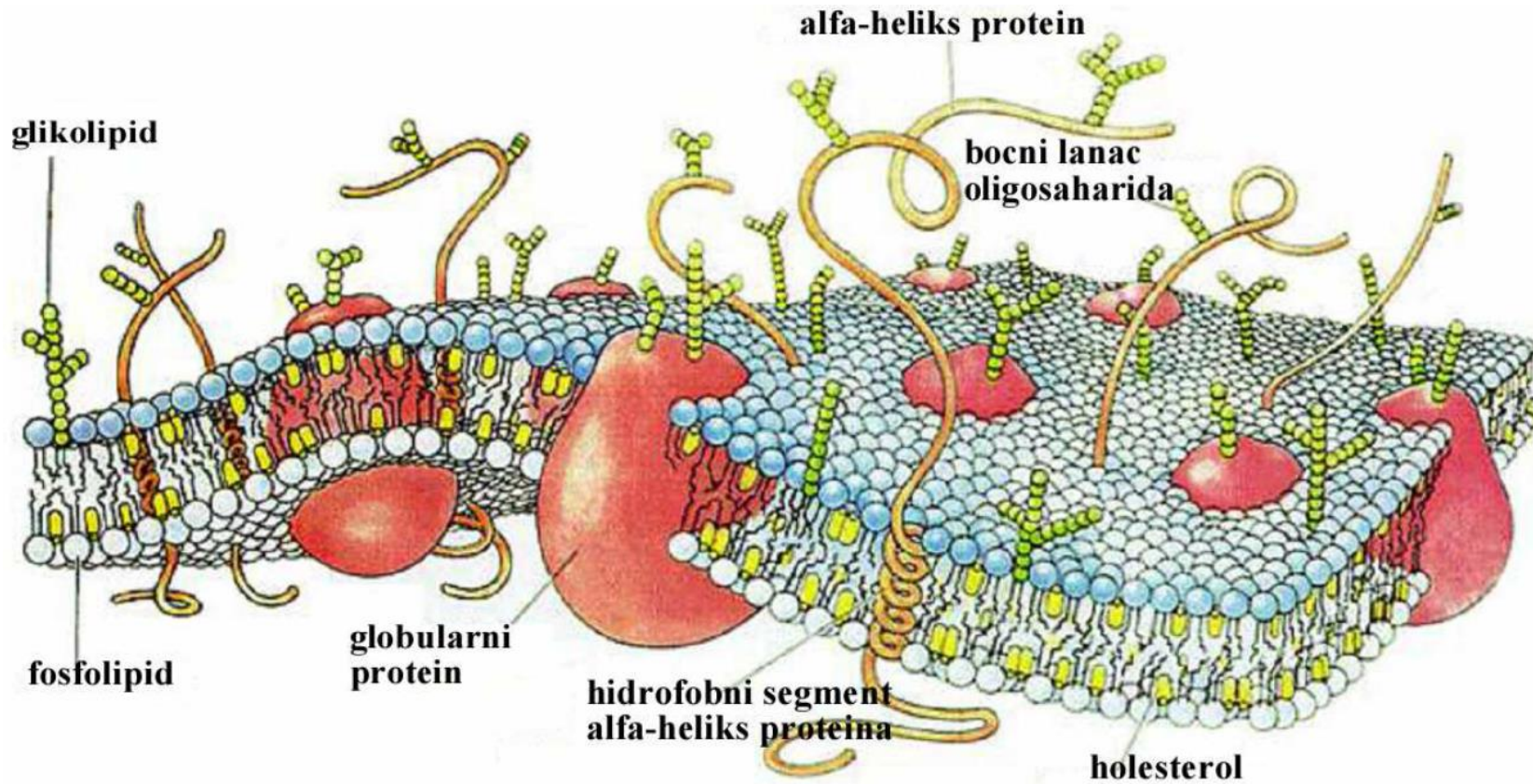


Vi-SEEM

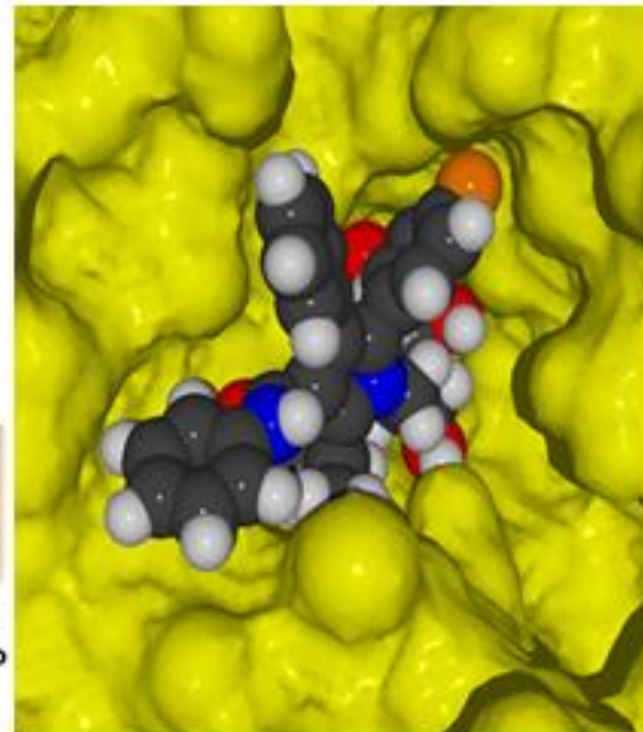
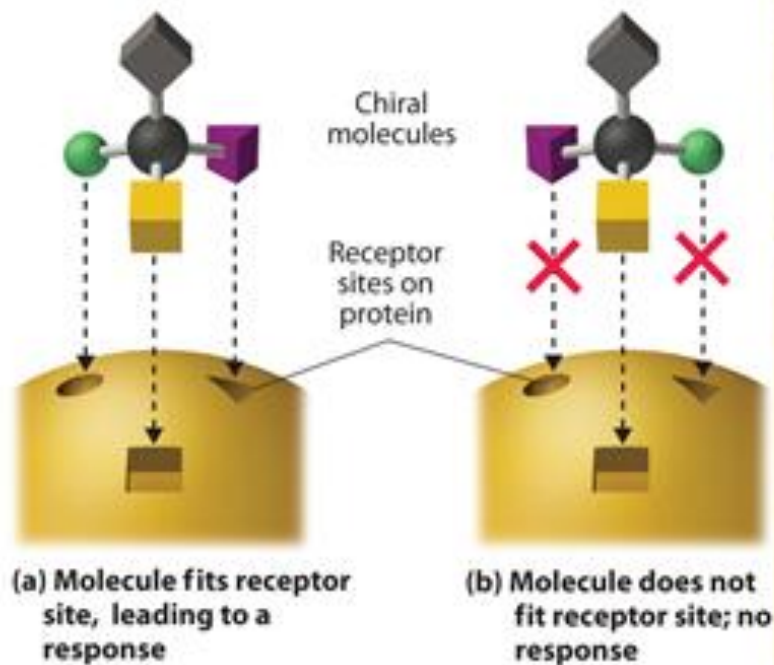
**XXII međunarodni
naučno-stručni skup
INFORMACIONE
TEHNOLOGIJE
Žabljak, 27.02.-04.03. 2017.**

Komparacija računarskog modela molekula sa eksperimentalnim rezultatima

□ INTERAKCIJA MOLEKULA I RECEPTORA

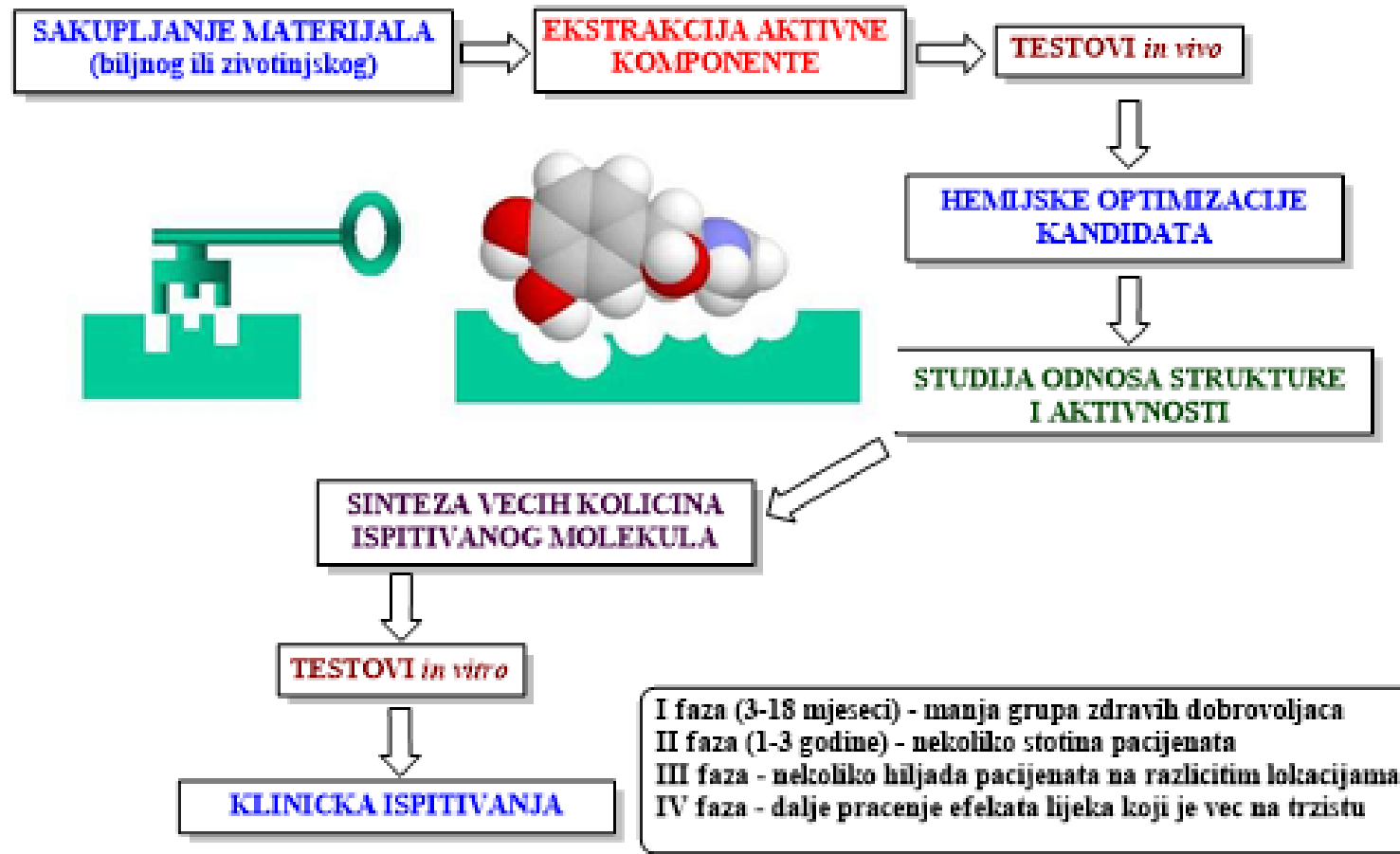


Stereo-elektronske osobine organskog molekula - lijeka



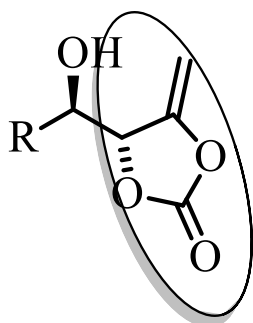
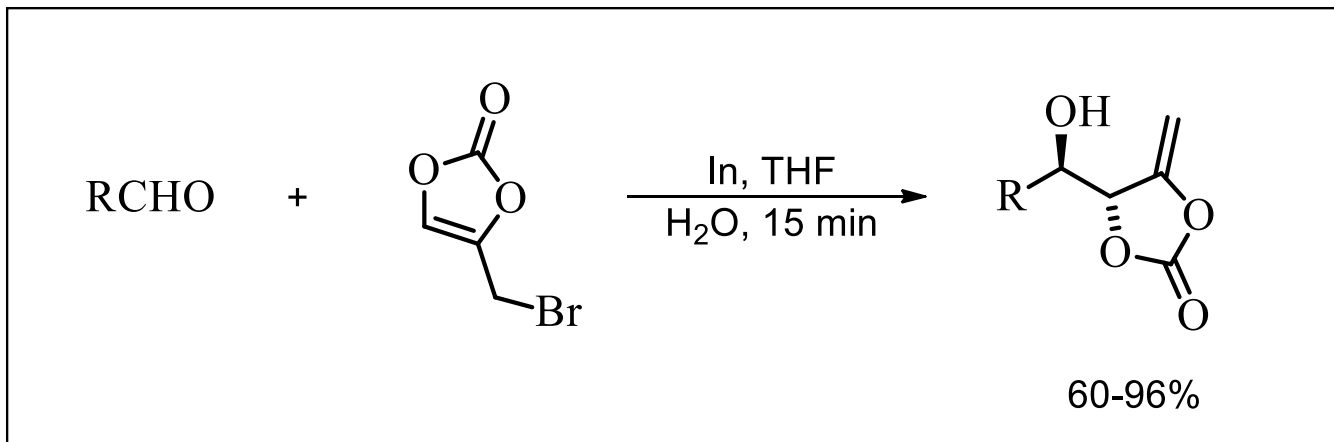
Komparacija računarskog modela molekula sa eksperimentalnim rezultatima

Faze razvoja novog lijeka

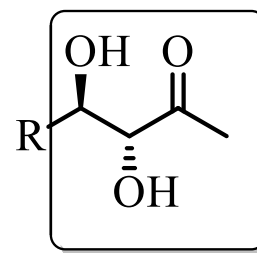


Komparacija računarskog modela molekula sa eksperimentalnim rezultatima

ENOL-KARBONATI KAO MOLEKULSKI MODELI ZA RAČUNARSKE SIMULACIJE

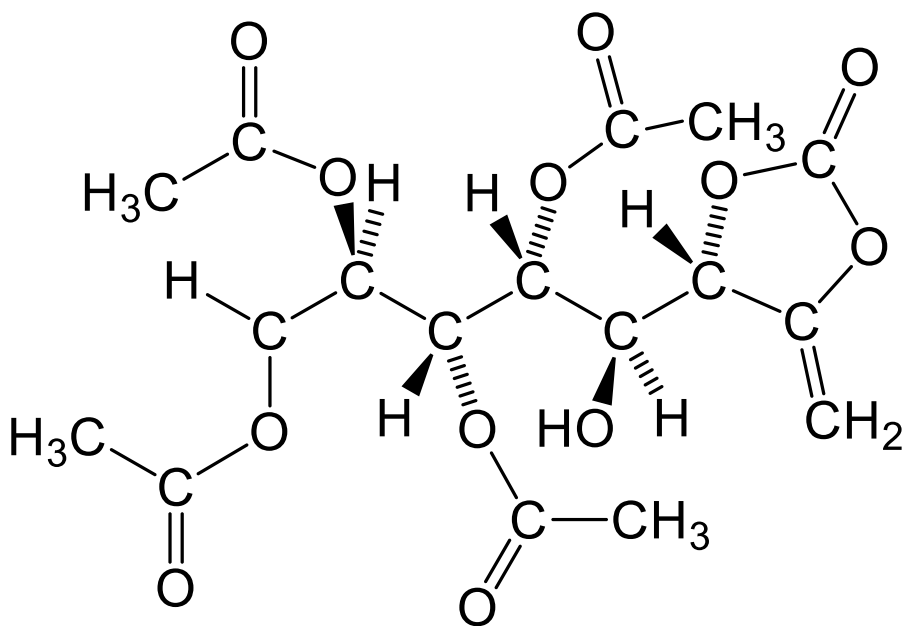


Enol-karbonatna forma

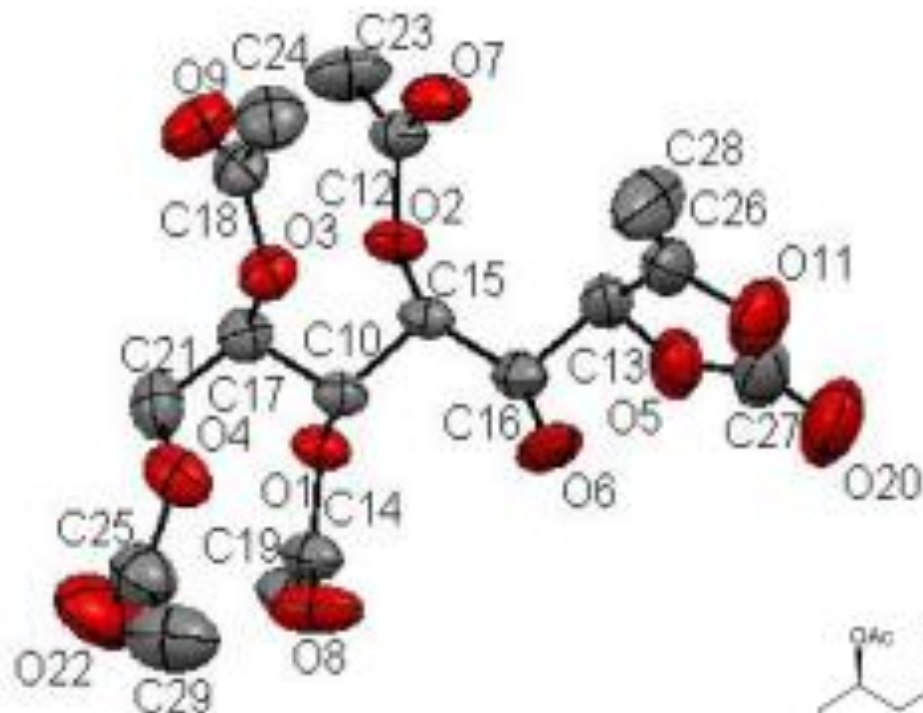


α,β -Diketonski fragment

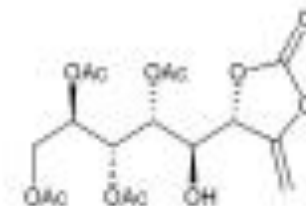
Komparacija računarskog modela molekula sa eksperimentalnim rezultatima



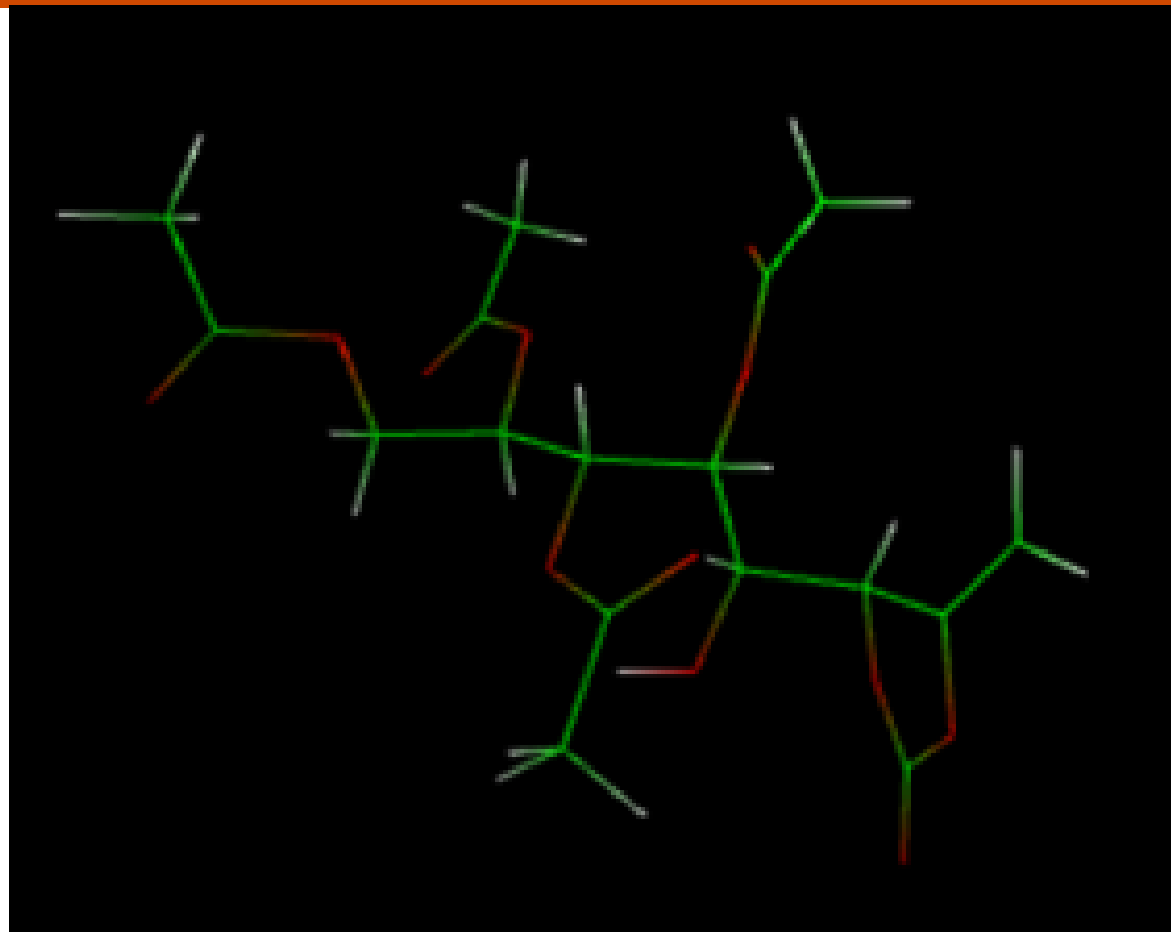
Strukturna formula (2R,3R,4R,5S)-5-hidroksi-5-((S)-5-metilen-2-okso-1,3-dioksolan-4-il)pentan-1,2,3,4-tetraacetata



RSA enol-karbonata



Komparacija računarskog modela molekula sa eksperimentalnim rezultatima



Izgled (2R,3R,4R,5S)-5-hidroksi-5-((S)-5-metilen-2-okso-1,3-dioxolan-4-il)pentan-1,2,3,4-tetraacetata u program VegaZZ (PDB format)

HVALA NA PAŽNJI!