

# **HEDEF (RESEPTÖR) KAYNAKLI İLAÇ TASARIMI**

**Hedeften hareketle 3-boyutlu ilaç tasarımı**

# DOCKING YÖNTEMİ

**MOLEKÜLÜN RESEPTÖR  
CEPLERİNE YERLEŐTİRİLMESİ  
YÖNTEMİ**

# DOCKING

Etkili olabilecek bileşik, Sterik ya da Elektrostatik yönden reseptördeki ceplere uygunluğu değerlendirilerek tasarlanır.

Protein (Reseptör) yüzeyi → Elektrostatik Potansiyeline göre renklendirilmiştir.

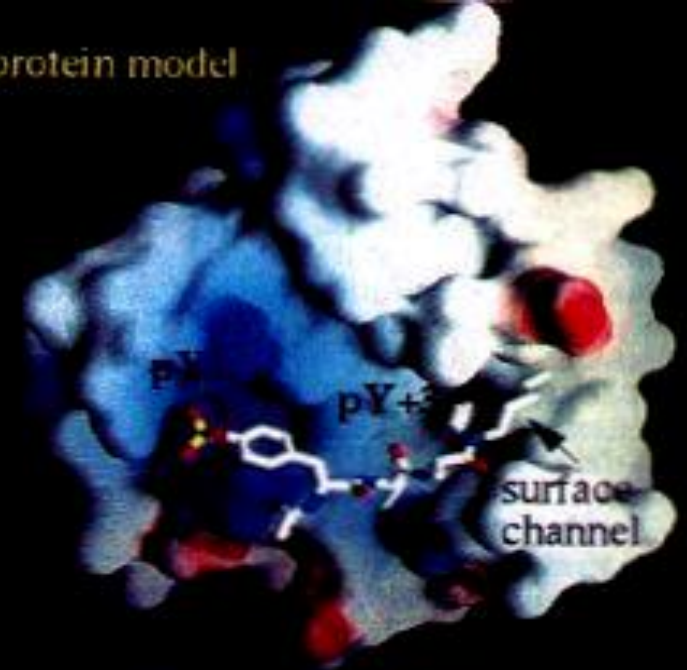
**Kırmızı** → Negatif;

**Mavi** → Pozitif

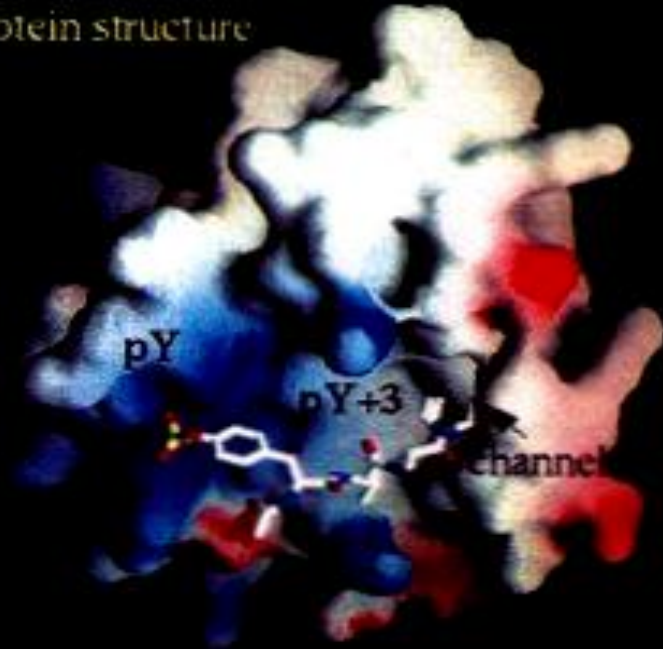
**PY cebi** → Elektropozitif;

**pY+3** → hidrofobik; hidrofobik kanal

(a) homology protein model

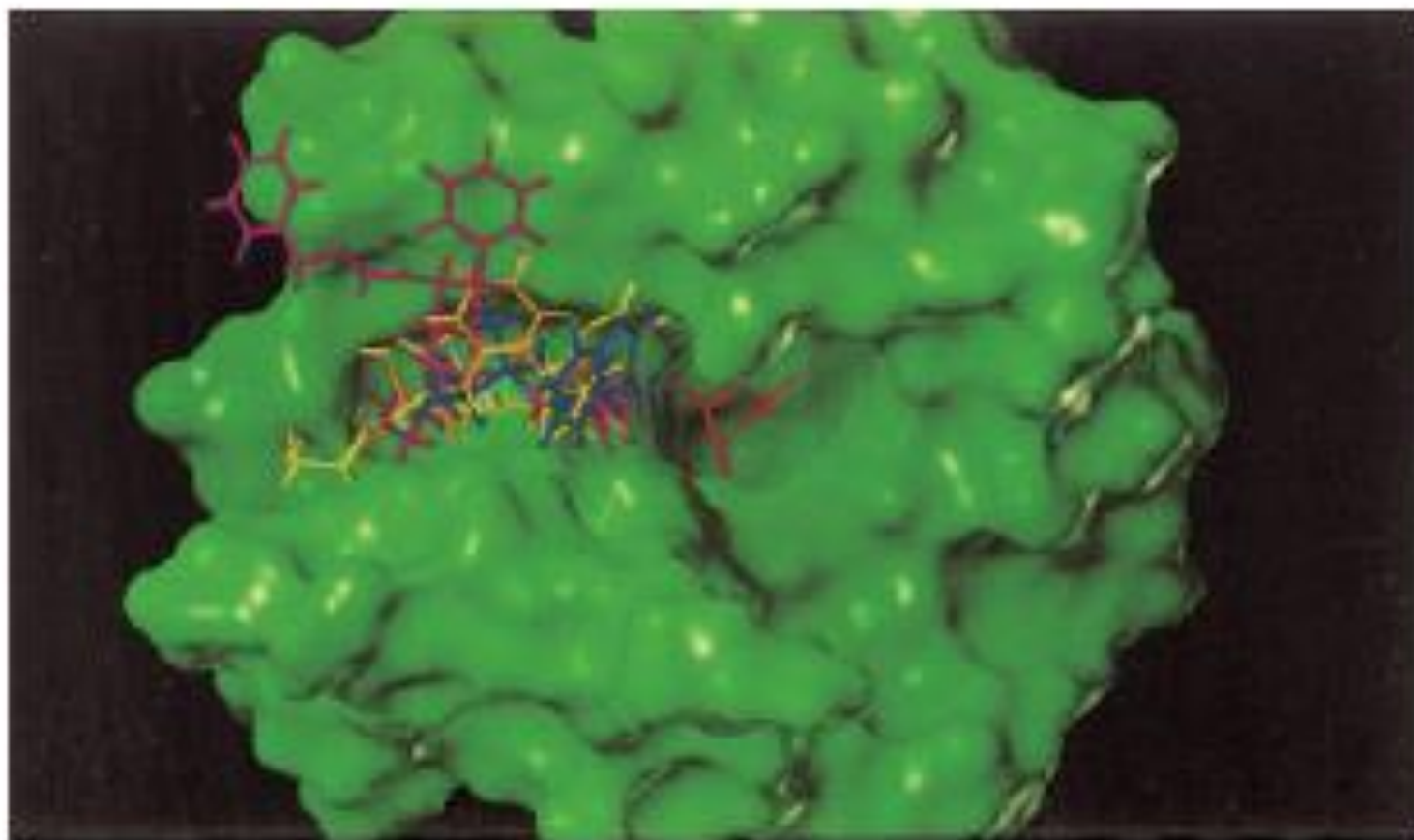


(b) published protein structure



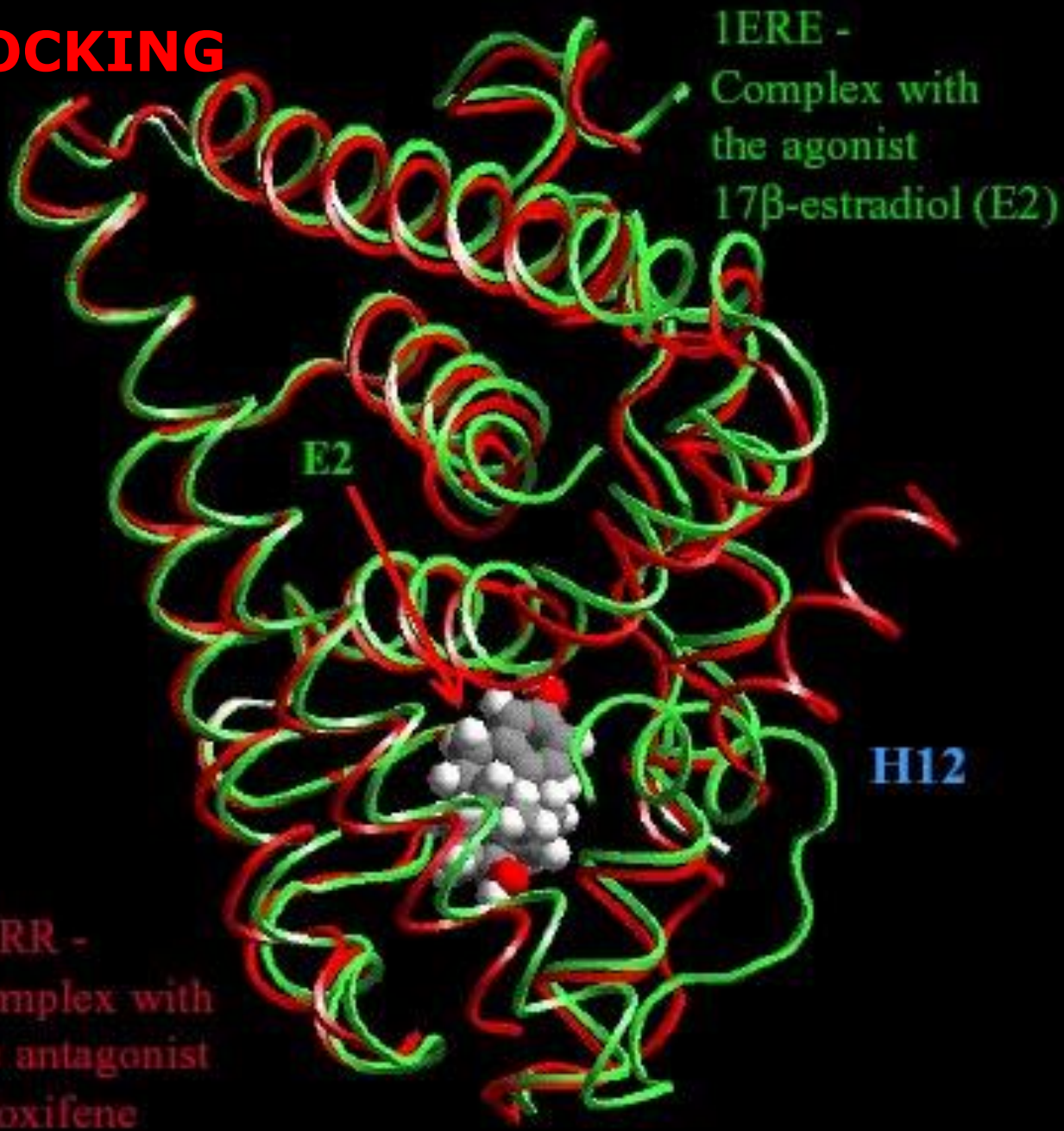
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*Kontoyianni, Sokol, and McClellan • Vol. 26, No. 1 • Journal of Computational Chemistry*



**Figure 2.** Inhibitors of thermolysin docked with FlexX. A representative ligand of a crystal complex is shown in red. The inhibitors are not docked as deeply into the pocket as the bound antagonist.

# DOCKING



IERR -  
Complex with  
the antagonist  
raloxifene

IERE -  
Complex with  
the agonist  
17β-estradiol (E2)

H12