

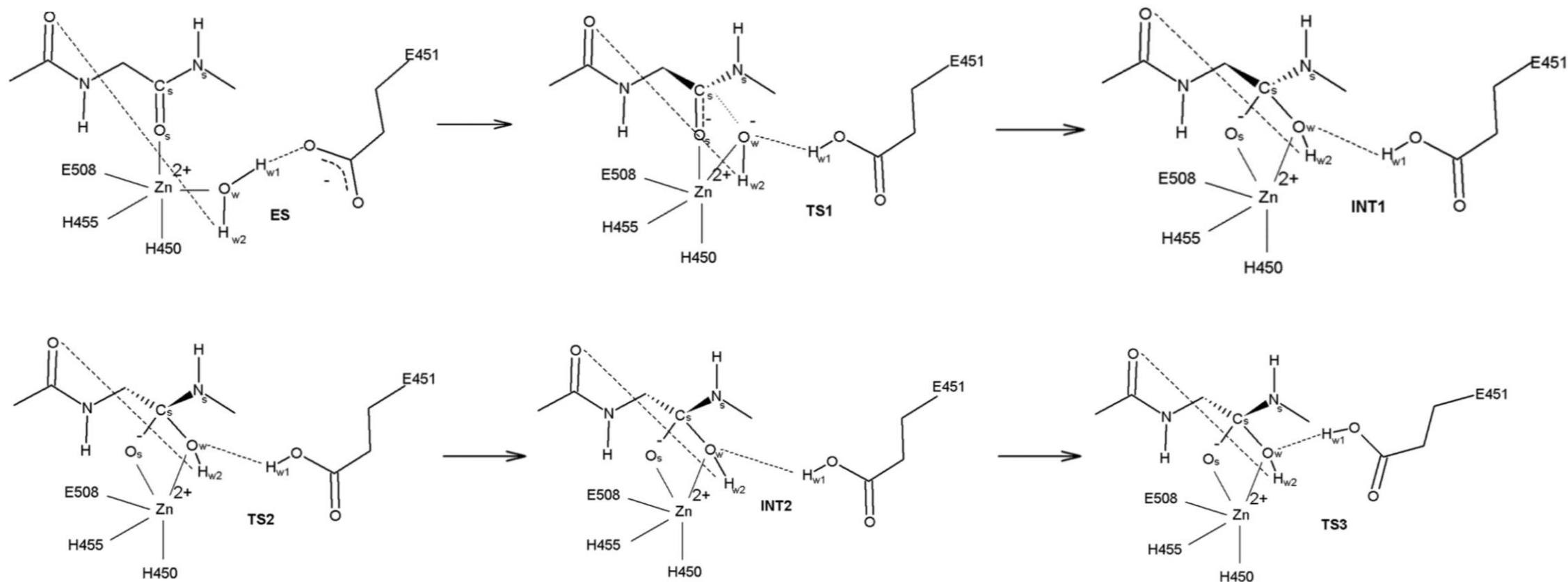
Istraživanje mehanizma hidrolize
peptidne veze na modelnom sustavu
DPP III iz *Bacteroides thetaotaomicron*

Marko Tomin

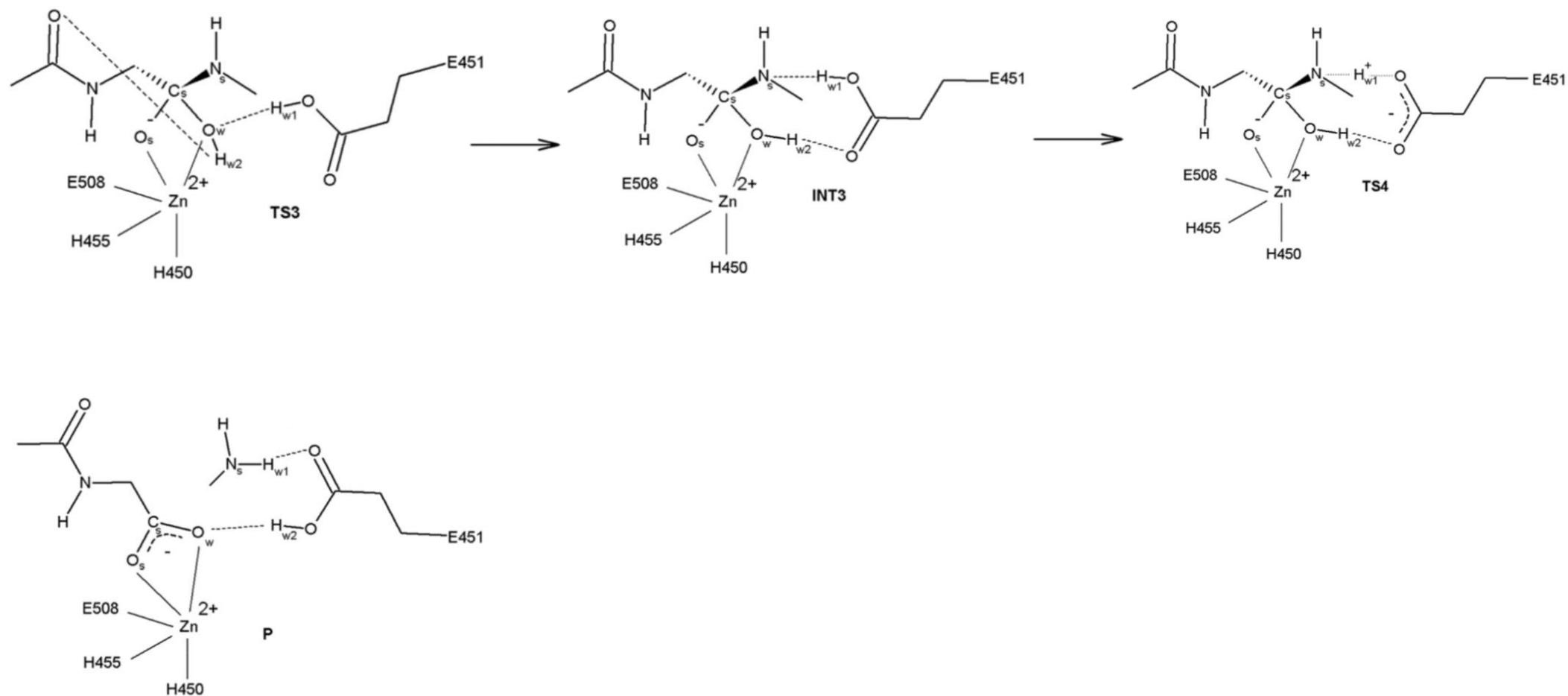
Mehanizam hidrolize humane DPP III

- Proučen na modelnom sustavu i cijelom enzimu¹
- Aktivacija molekule vode Glu451 te nukleofilni napad na karbonilni ugljik

Mehanizam h.DPP III (modelni sustav)

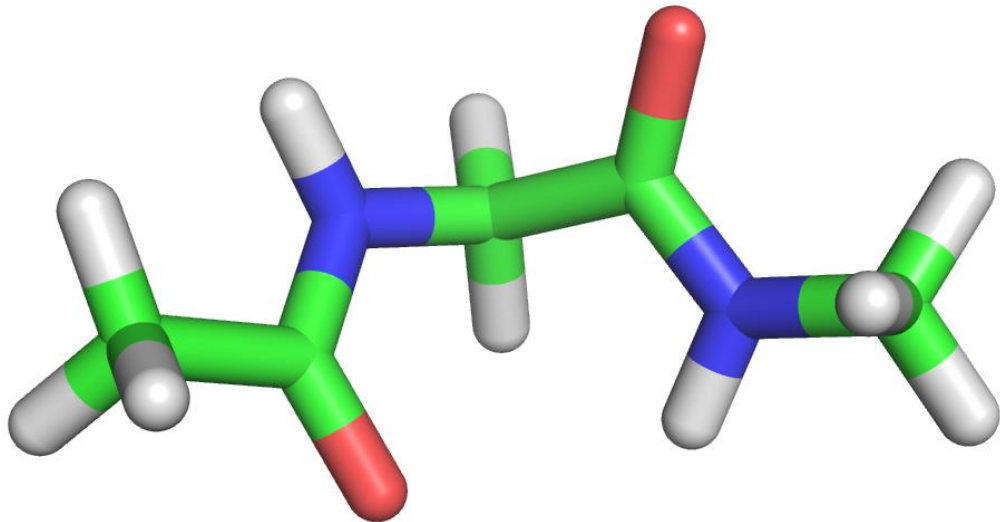


Mehanizam h.DPP III (modelni sustav)



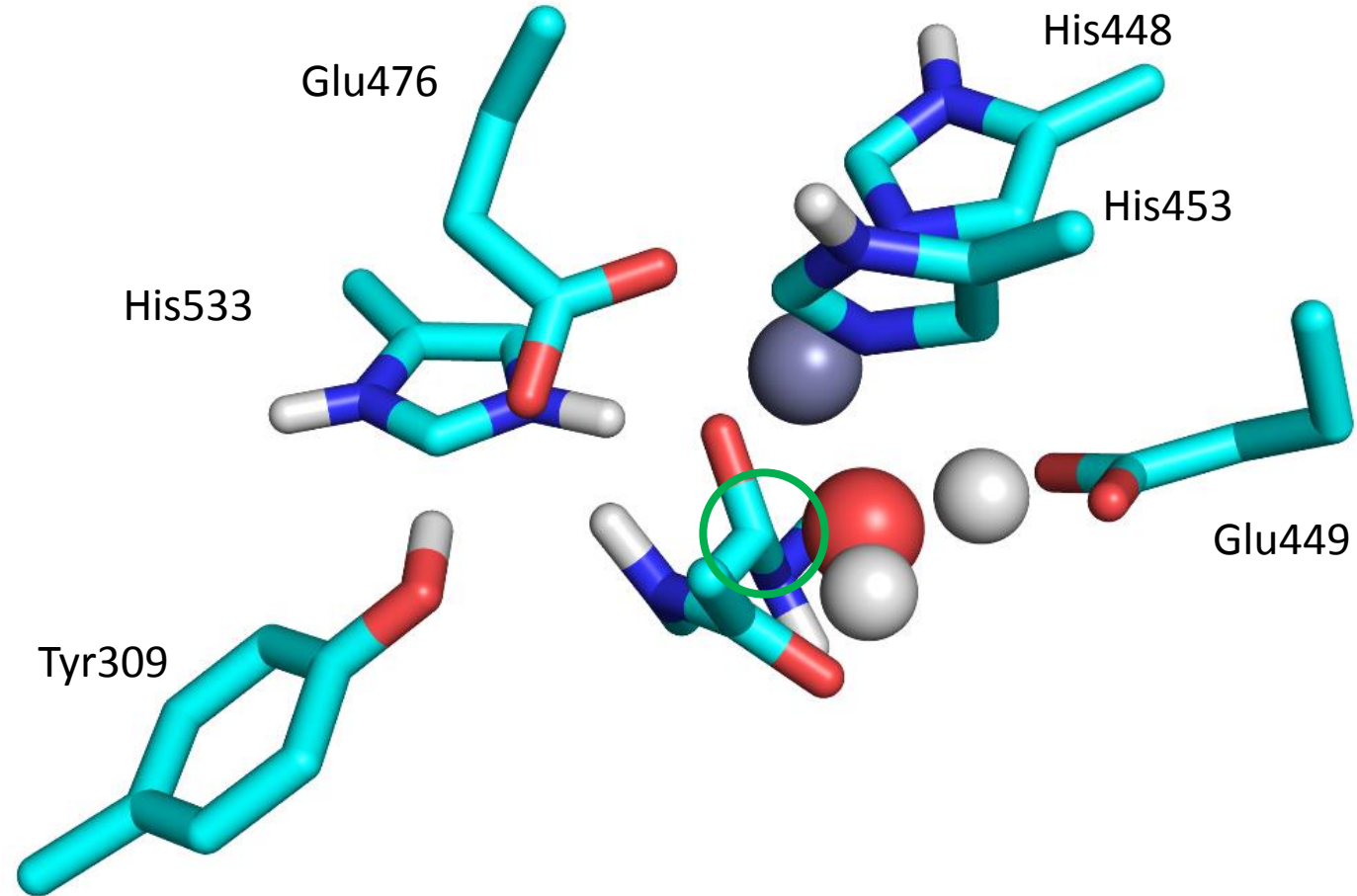
Modelni sustav *BtDPP* III

- Priređen iz rezultata molekulske dinamike (dokiranja)
- Korišteni kristalografska voda i Glu449

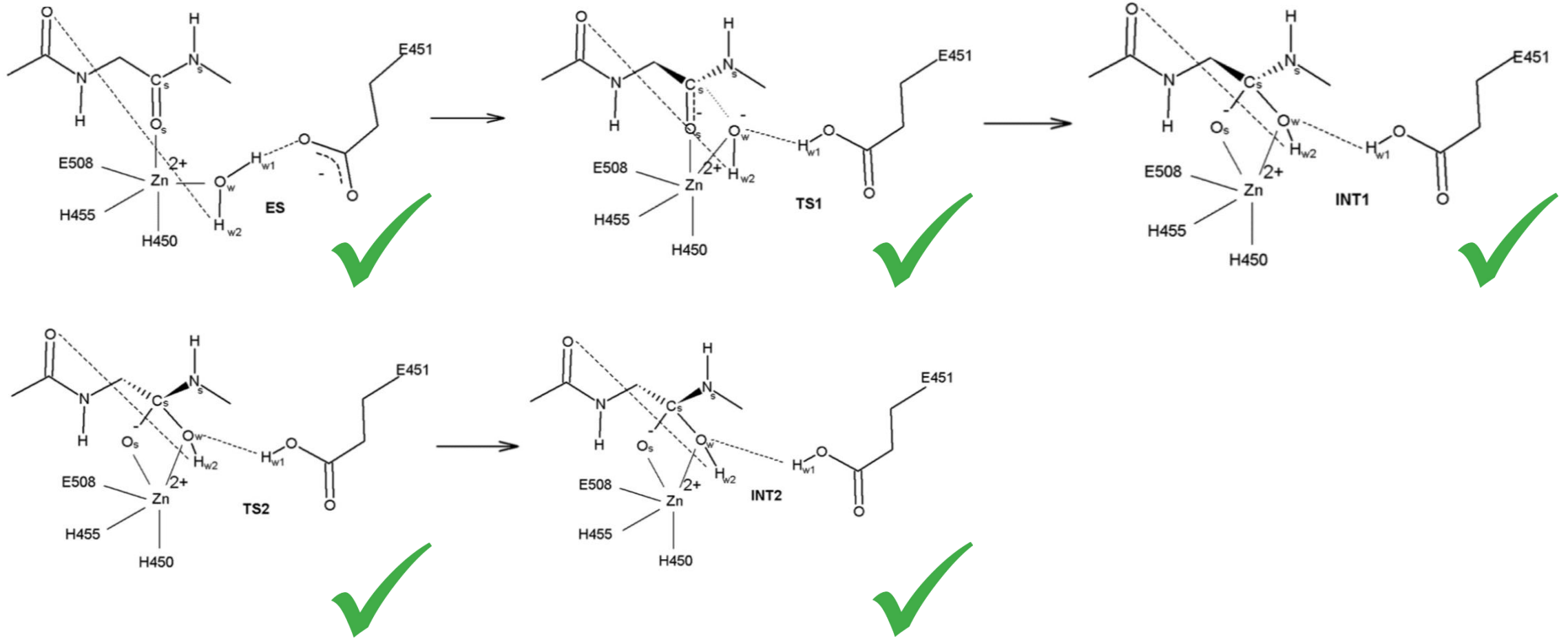


Polazna struktura kompleksa

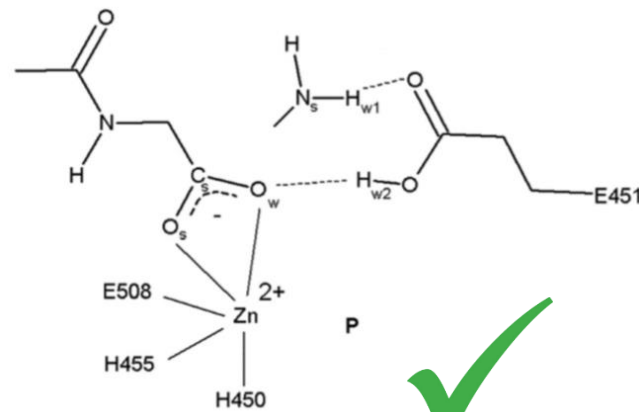
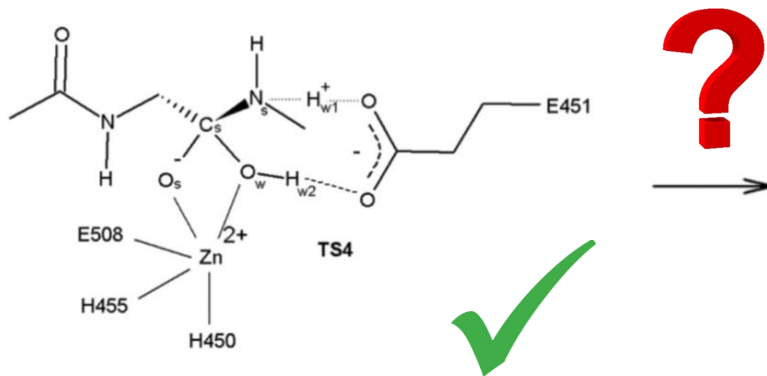
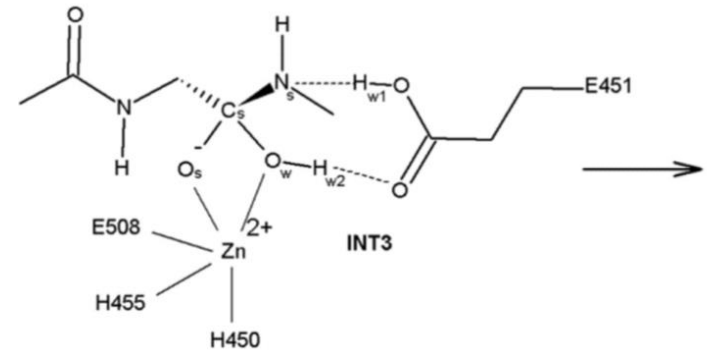
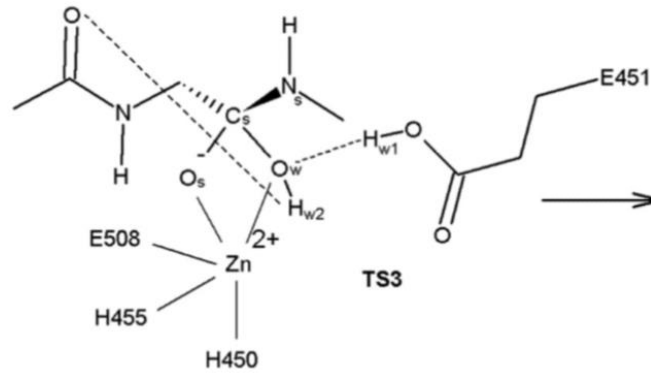
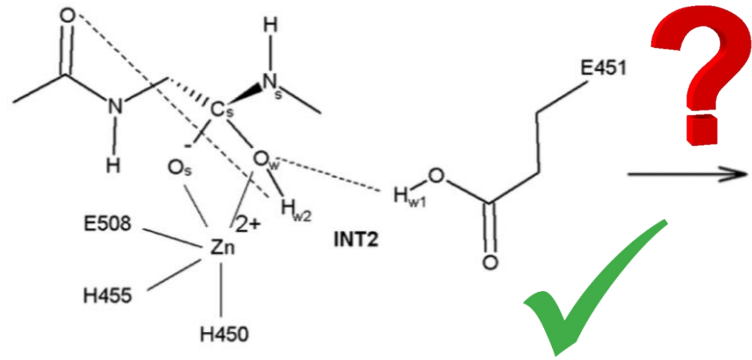
- Fiksirane točke



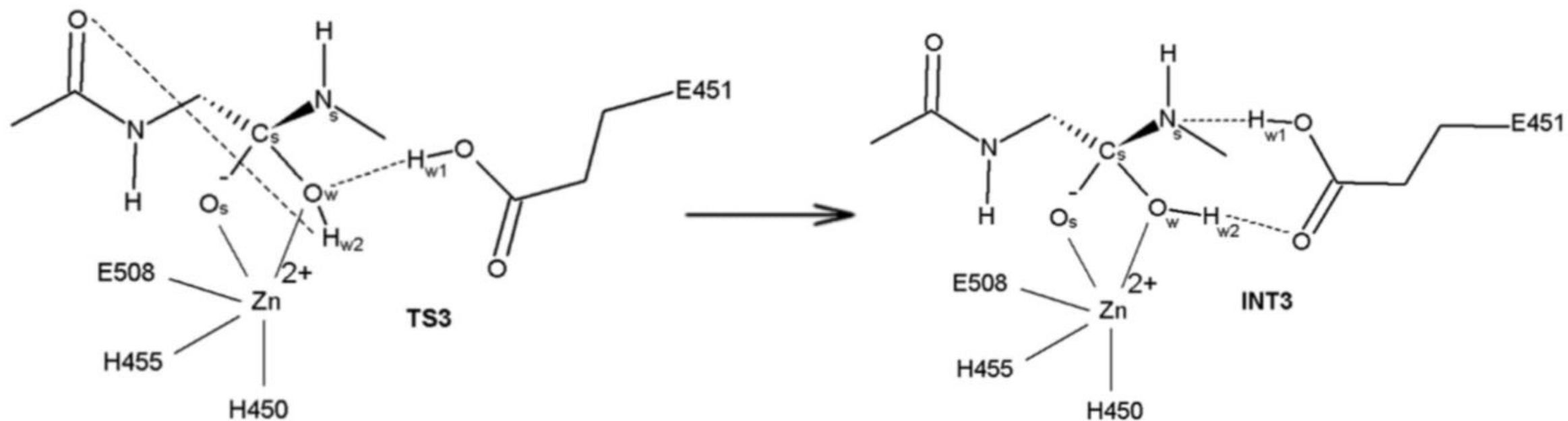
Rezultati



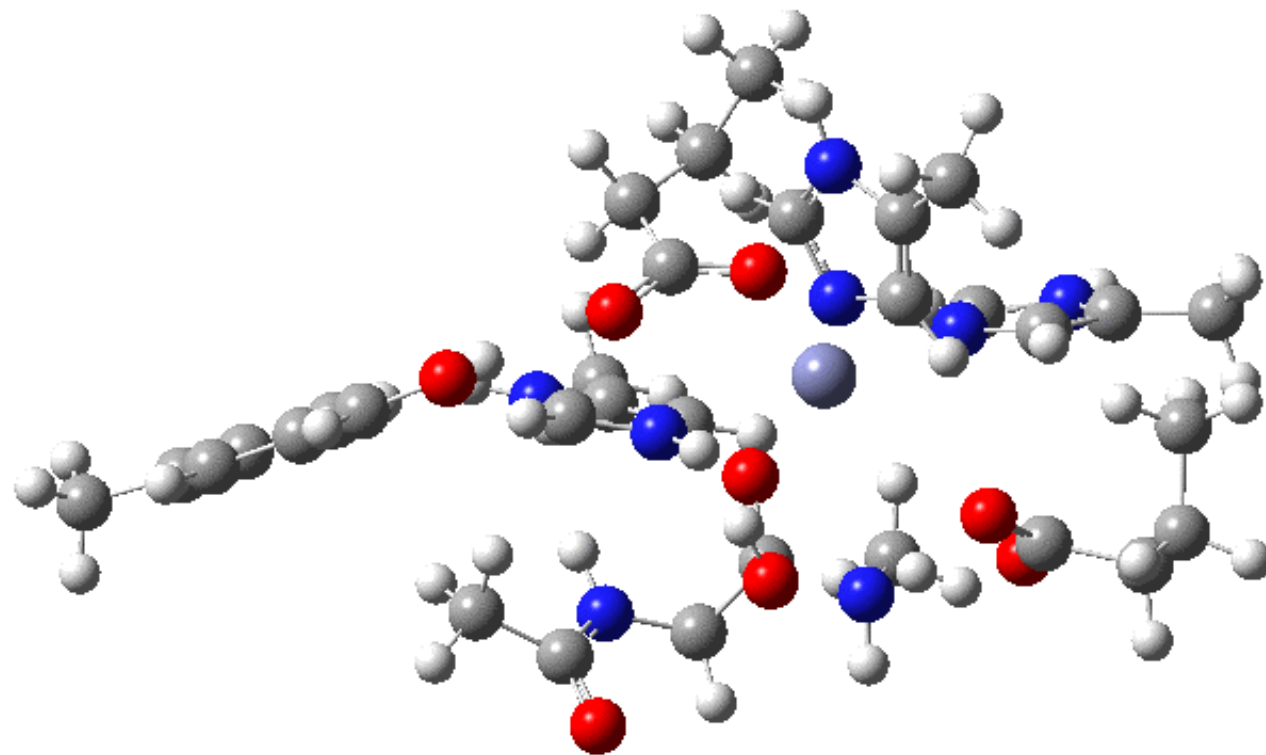
Rezultati



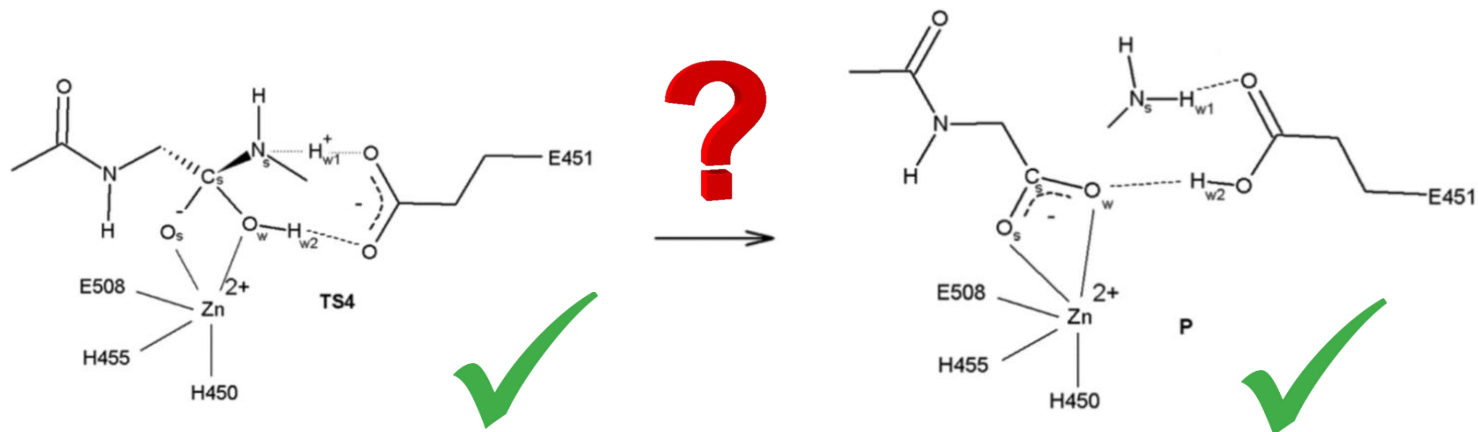
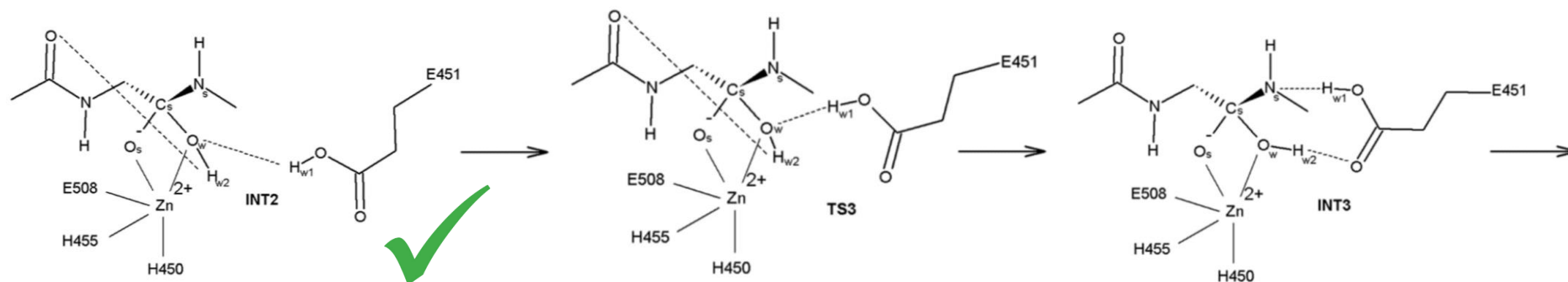
Konformacijska promjena – „zaključavanje”



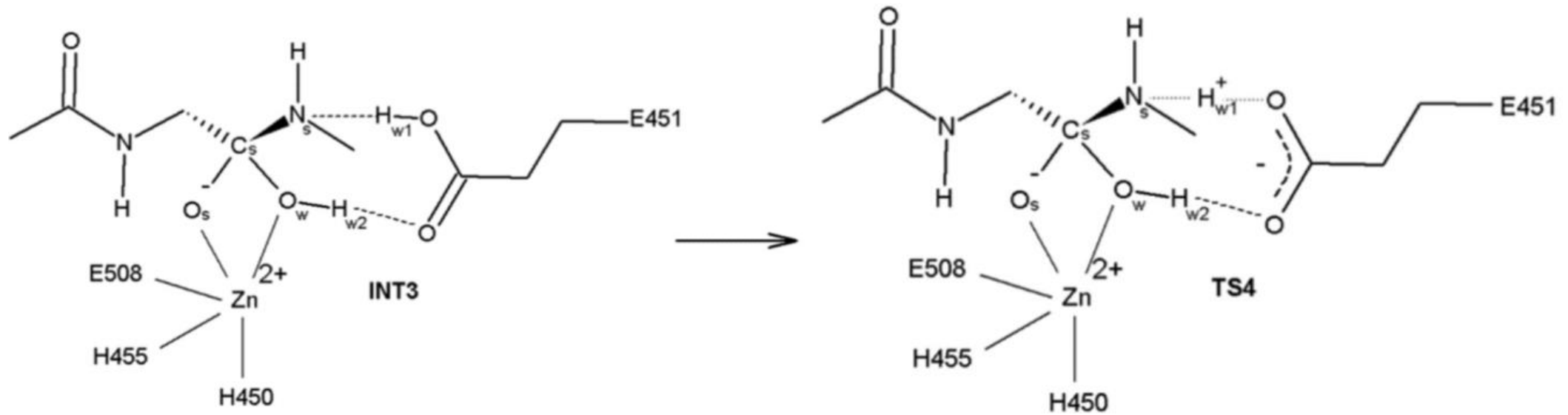
Rotacija vodikove veze



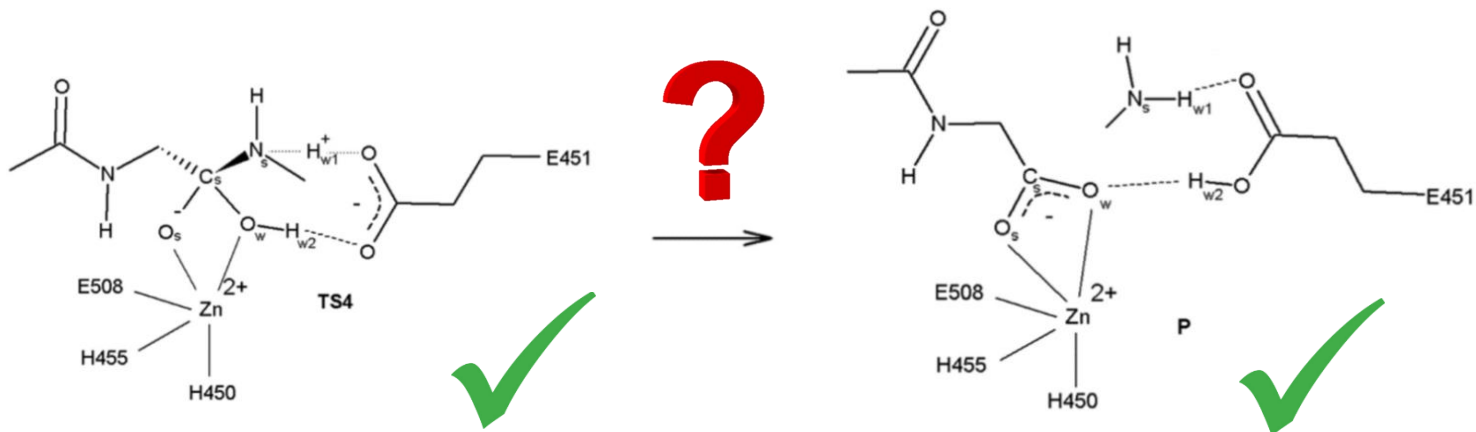
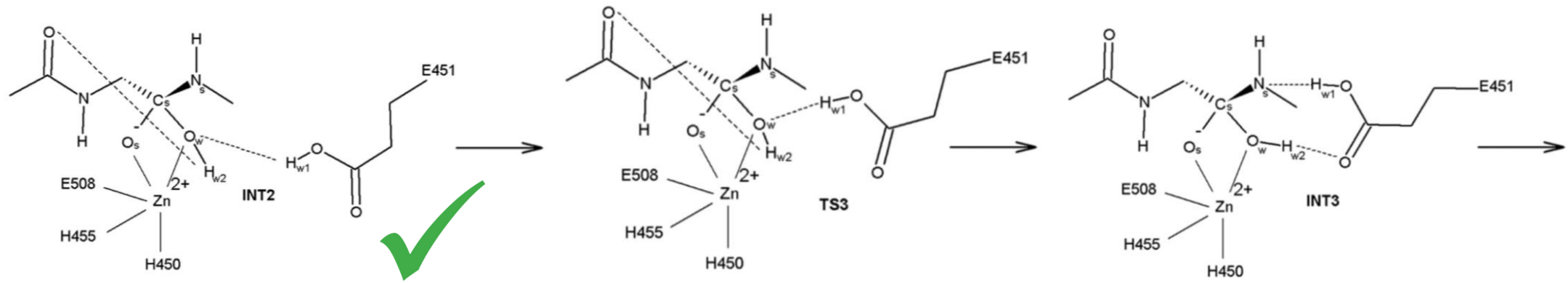
Rezultati



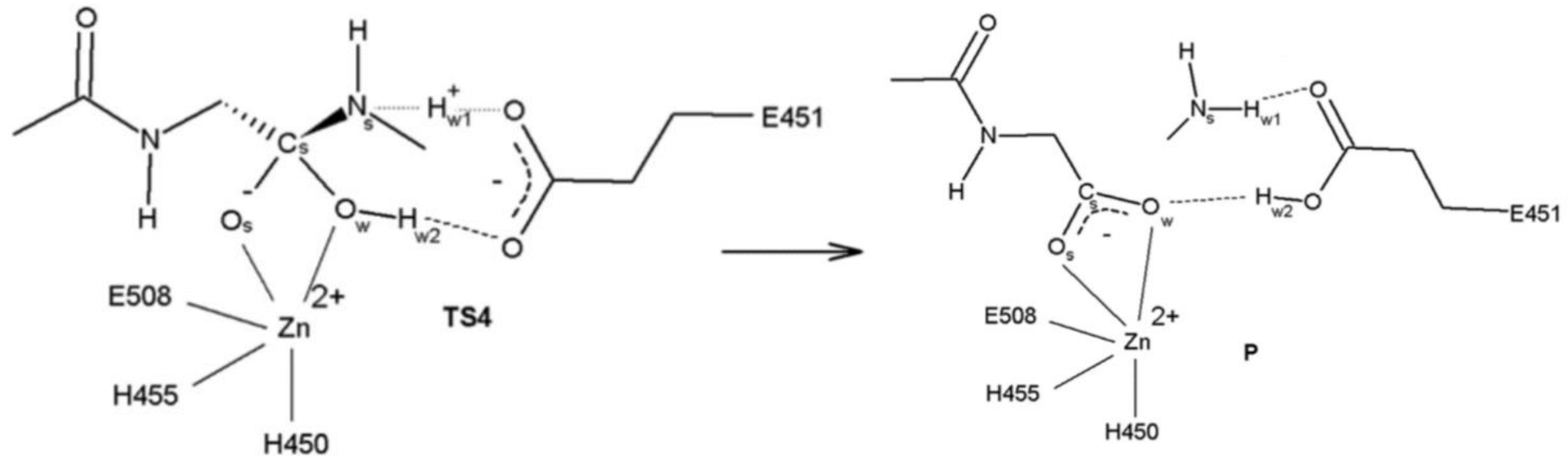
Prijenos protona



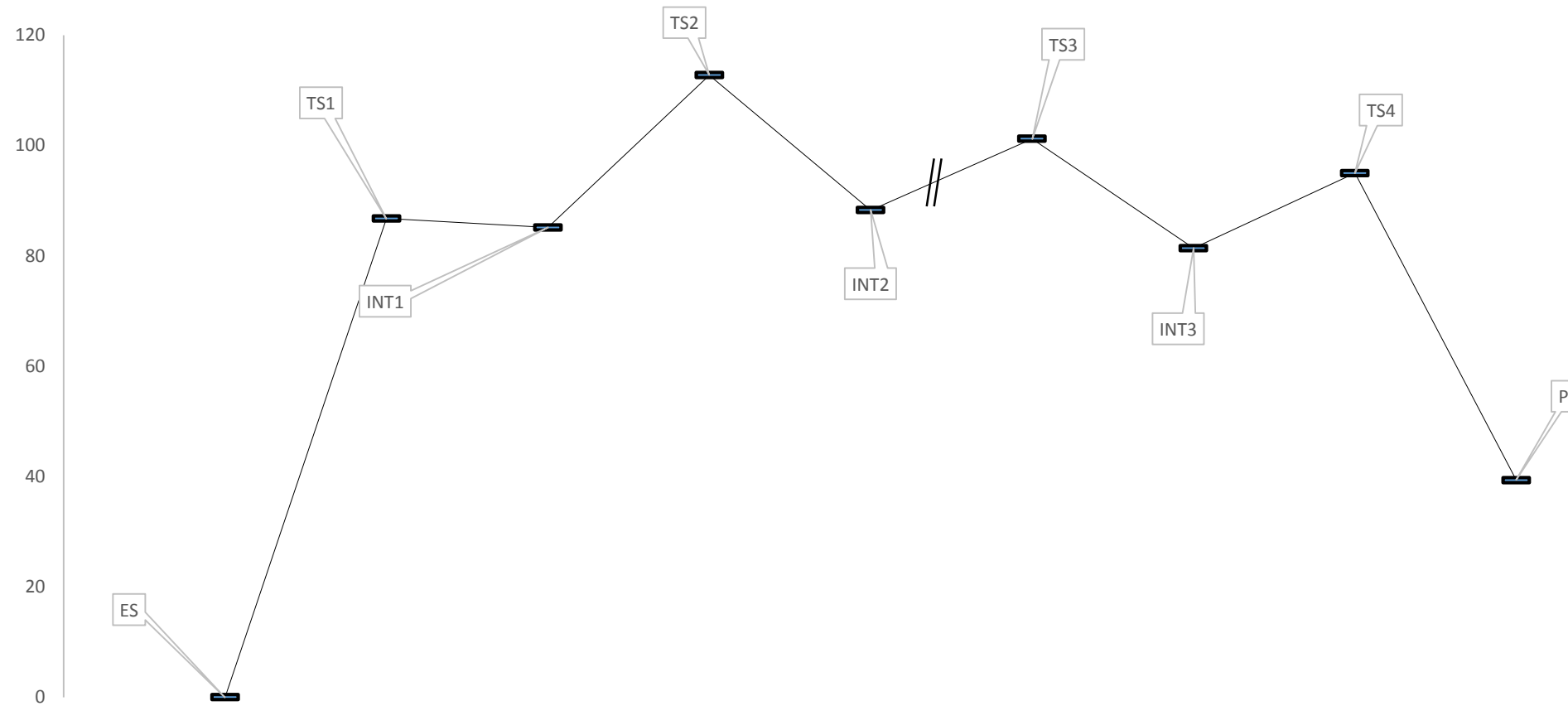
Rezultati



Nastanak produkata



Energije



Budući planovi

- QM/MM pristup
 - Nestanak problema male konformacijske promjene
- Bolji energetska profil reakcije
 - Fiksirane točke – loša rezolucija polazne strukture

Zahvale



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Dr. sc. Antonija Tomić



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- Ana Tomašić Paić
- Marina Grabar Branilović
- Mihaela Matovina
- Sara Matić
- Snježana Jurić
- Zrinka Karačić



Hvala na pažnji!