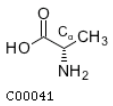
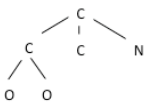
A.



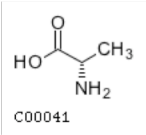


$^0\sigma(C_\alpha)$ = [C]()

$^1\sigma(C_\alpha)$ = [C]([C][C][N])

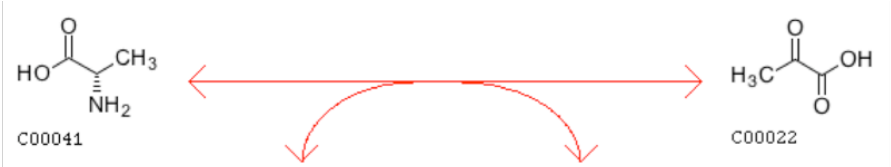
$^2\sigma(C_\alpha)$ = [C]([C][C]([O]=[O])[N])

B.

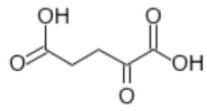


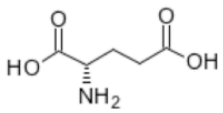
$^2\sigma(C_{41})$ = 1 [C]([C]([C][N]))
1 [C]([C]([C][N])[O]=[O])
1 [C]([C][C]([O]=[O])[N])
1 [N]([C]([C][C]))
1 [O](=[C]([C][O]))
1 [O]([C]([C]=[O]))

C.



1 [C]([C]([C][N]))
1 [C]([C]([C][N])[O]=[O])
1 [C]([C][C]([O]=[O])[N])
1 [N]([C]([C][C]))
1 [O](=[C]([C][O]))
1 [O]([C]([C]=[O]))





1 [C]([C]([C])[C]([C]=[O]))
1 [C]([C]([C])[C]([O]=[O]))
1 [C]([C]([C])[C]([O]=[O])=[O])
1 [C]([C]([C])[O]=[O])
1 [C]([C]([C]=[O])[O]=[O])
1 [O](=[C]([C][C]))
2 [O](=[C]([C][O]))
2 [O]([C]([C]=[O])))

1 [C]([C]([C])[C]([C][N]))
1 [C]([C]([C])[C]([O]=[O]))
1 [C]([C]([C])[C]([O]=[O])[N])
1 [C]([C]([C])[O]=[O])
1 [C]([C]([C][N])[O]=[O])
1 [N]([C]([C][C]))
2 [O](=[C]([C][O]))
2 [O]([C]([C]=[O]))

$^2\sigma(EC\ 2.6.1.2) = {}^2\sigma(C_{22}) + {}^2\sigma(C_{25}) - {}^2\sigma(C_{41}) - {}^2\sigma(C_{26}) =$

1 [C]([C][C]([O]=[O])=[O])
1 [C]([C]([C]=[O]))
-1 [C]([C]([C][N]))
-1 [C]([C]([C])[C]([C]=[O]))
-1 [C]([C][C]([O]=[O])[N])
1 [C]([C]([C])[C]([C][N]))
1 [C]([C]([C])[C]([O]=[O])[N])
-1 [C]([C]([C])[C]([O]=[O])=[O])

Figure S1. How to compute the atomic, molecular, and reaction signatures for the alanine transaminase (EC 2.6.1.2). **A)** Atomic signature of alanine C_α of heights h = 0,1, and 2; **B)** Molecular signature of height h = 2 of alanine. **C)** Reaction signature of height h = 2 of alanine transaminase, computed as the difference between the signatures of the substrates and the signatures of the products.