

Supplementary Information

The Reaction Mechanism of Cathepsin A and the Effect of Protonation States of pH Regulators and the Substrate: A Cluster Modelling DFT Study

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S1. Model Calculations of Enzyme Reaction with Model 1

The first model study built included an imidazole in place of His429, a methanol in place of Ser150 and a formamide in place of substrate. The oxyanion hole and Asp372 amino acids are not represented in this very simple model. The reaction mechanism is very similar to literature mechanism where first step is from M1-1 to first step's product. First step's product, however, is slightly different from second step's reactant (M1-2). It is seen that proton transfer from imidazole to scissile -NH₂ is required before second (peptide bond hydrolysis) step since negative charge accumulation on nitrogen is harder than oxygen. Thus, unlike steps 1, 3 and 4, the nitrogen of scissile N-C bond at step 2 has to be protonated prior to reaction, for M1 model. After second step, the product M1-3 is converted to M1-3W by removing ammonia and putting water in its place. Third step reaction occurs in a concerted fashion as well, obeying the literature mechanism, as well as the fourth step reaction. The structures and relative Gibbs Free Energies of the smallest M1 model are depicted below.

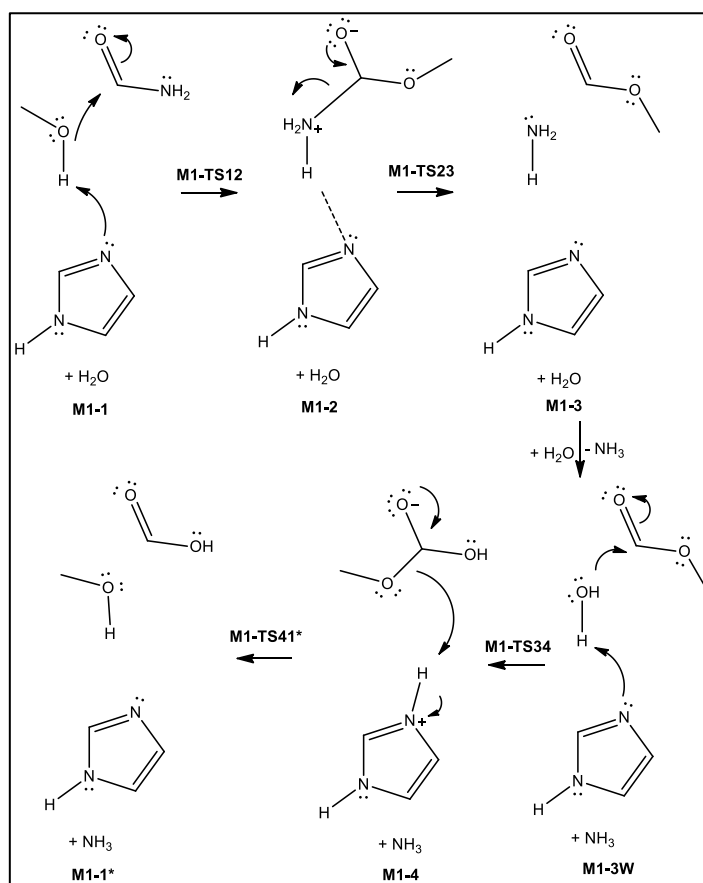
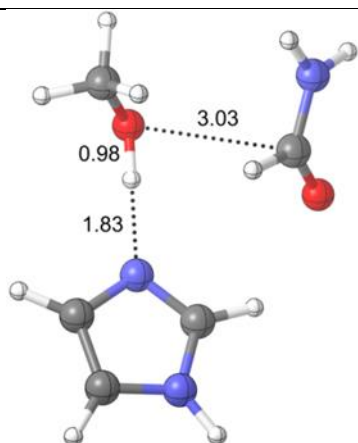
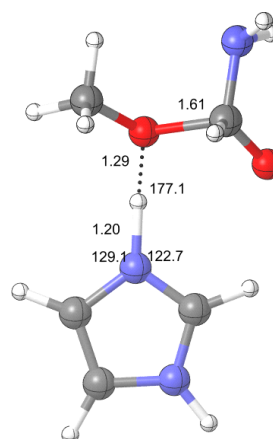


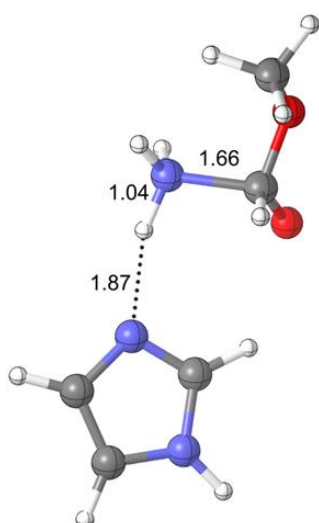
Figure S1. The smallest model (Model 1) for the carboxypeptidase reaction of CatA.



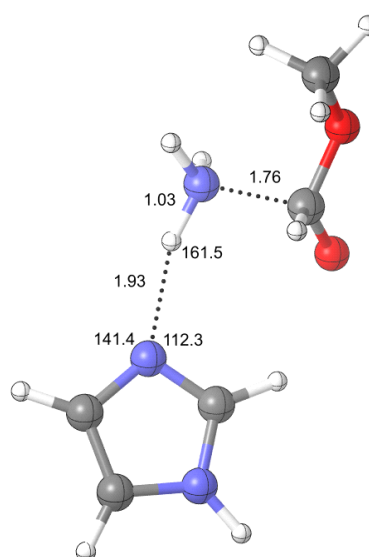
M1-1: 0.00 kcal/mol



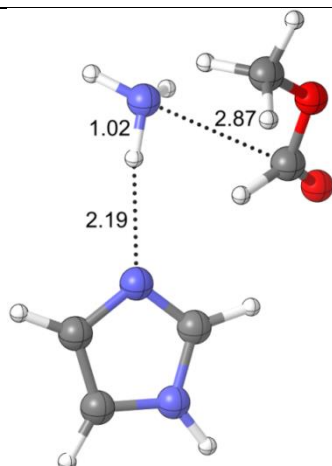
M1-TS12: 29.72 kcal/mol



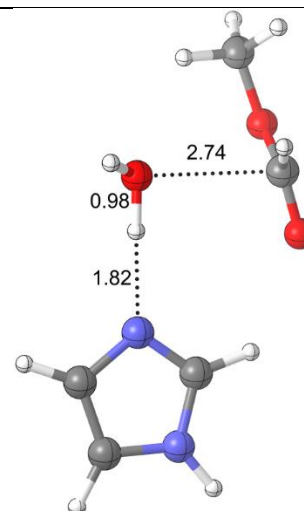
M1-2: 22.19 kcal/mol



M1-TS23: 21.06 kcal/mol



M1-3: 6.89 kcal/mol



M1-3W: 3.18 kcal/mol

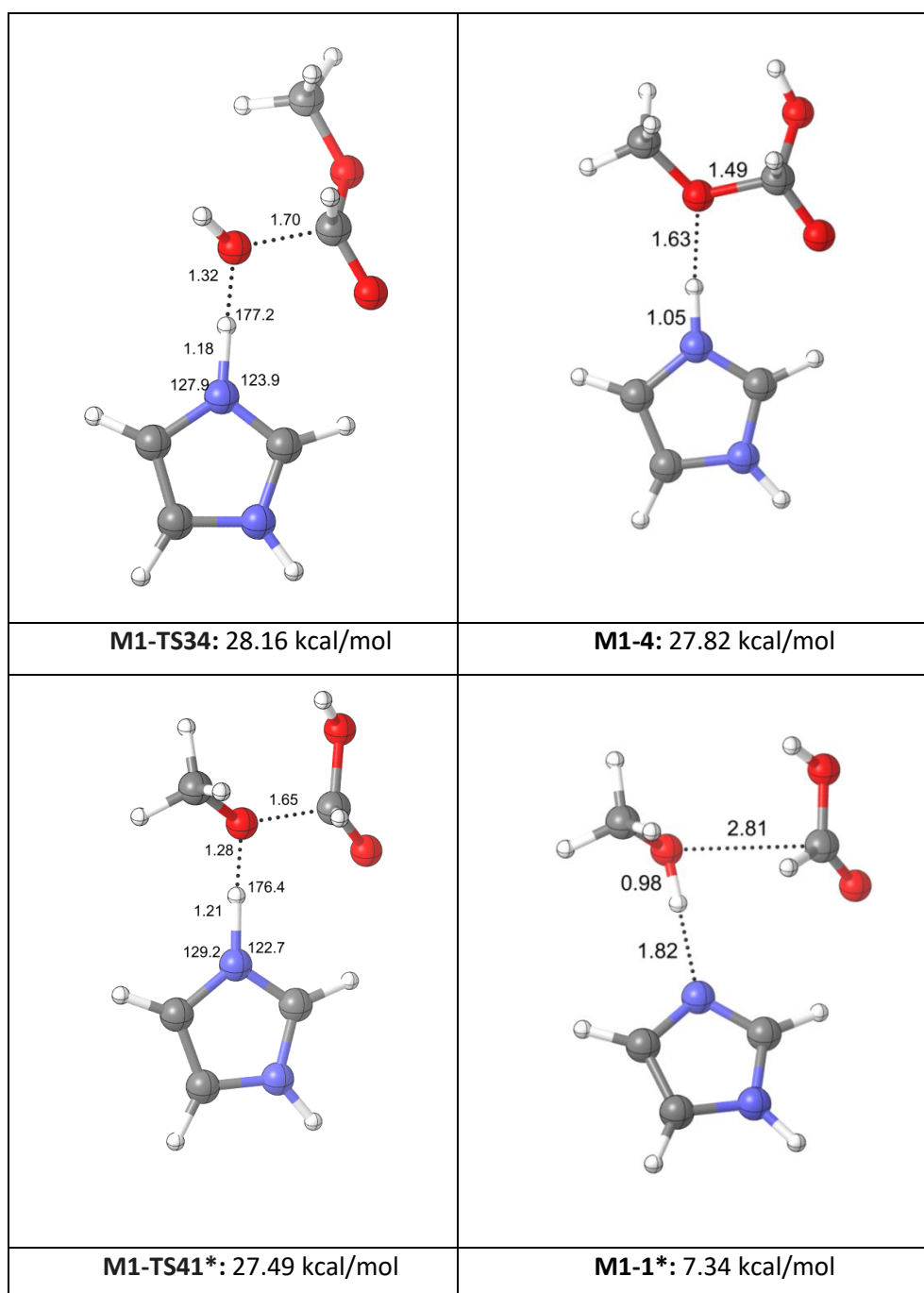


Figure S2. The 3-dimensional geometries (intermediates and transition state structures) of the reaction mechanism of the first model study. (Energies are relative Gibbs Free Energies in kcal/mol)

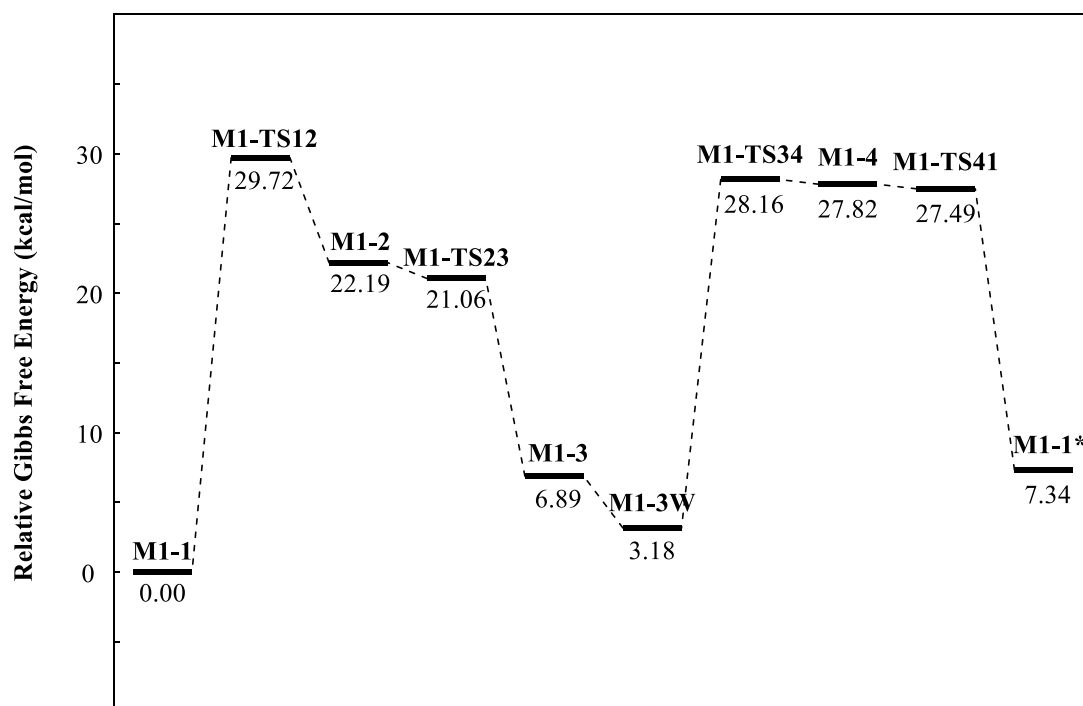


Figure S3. Reaction profile of M1 model study. (Energies are relative Gibbs Free Energies in kcal/mol)

S2. Model Calculations of Serine Carboxypeptidase Reaction with Model 2.

In the next model (referred as M2), N-methylacetamide is used as the substrate and Asp372 is modelled as an acetate. Ser150 (side chain, alpha carbon and C-end) along with Tyr151 (N end and alpha carbon) are taken as nucleophile of catalytic triad and oxyanion hole amino acid, respectively. His429 is represented as imidazole. Gly56 alpha carbon and the C-end along with Gly57 N-end and alpha carbon are considered in the model study to properly represent the other H donor to the oxyanion hole. The aminoacid counterparts of the model are mostly taken from their exact positions at their X-ray data (pdb code: 4cia) to initiate reaction. The place of reacting centers were adjusted so as to model the first step of the reaction where activation of Ser takes place. The transition state **M2-TS12** of first step had a barrier (relative Gibbs Free Energy) of 19.22 kcal/mol while the reaction product **M2-2** had a relative Gibbs Free energy of 19.02 kcal/mol. Modelling further reaction from the first step product was challenging. It is worth noting here that two proton transfer mechanism is clearly observed for step 1 of the reaction. As His429 attacked Ser150 proton, Asp372 attacked the other His429 proton in this model. The geometry of the model was significantly distorted for step 2 where amide bond (N-C) needed to break. Retaining position of all atomic centers but switching Ser150 side chain oxygen and substrate's NH locations led a modification, however this modification was required for a geometrically applicable structure for step 2 reaction (**M2-2***). After geometric restrictions for modelling step 2 transition state were overcame, same electronic restriction that was observed in step 2 of M1 model observed for M2 model as well: nitrogen had to be protonated prior

to the cleavage of peptide bond. When His-H proton is moved to scissile amide NH manually it was observed that the proton that moved from His429 to Asp372, moved back to imidazole group, preventing an anionic imidazole ring to occur. For that, it is worth mentioning that two proton transfer mechanism is also observed for step 2 of M2 model. This new system (double proton transfer from M2-2*) is named as **M2-2**** and it has a relative Gibbs Free Energy of 21.89 kcal/mol. Then, the transition state of step 2 was modeled and **M2-TS23** had a relative Gibbs Free Energy of 21.31 kcal/mol. After step 2 transition state, the system could not be modeled further because forward irc of transition state of **M2-TS23** significantly collapsed and curled into a ball-like structure without geometric restrictions inherent to the enzyme. Therefore, this structure and the steps after this structure considered as not applicable to model.

In the second model study, it is observed that inclusion of Asp372 and oxyanion hole decreases the first step reaction barrier by 10.50 kcal/mol (with respect to the first step of M1 model). In M2 model, it is also observed that two proton transfer mechanism is dominant in step 1 and step 2.

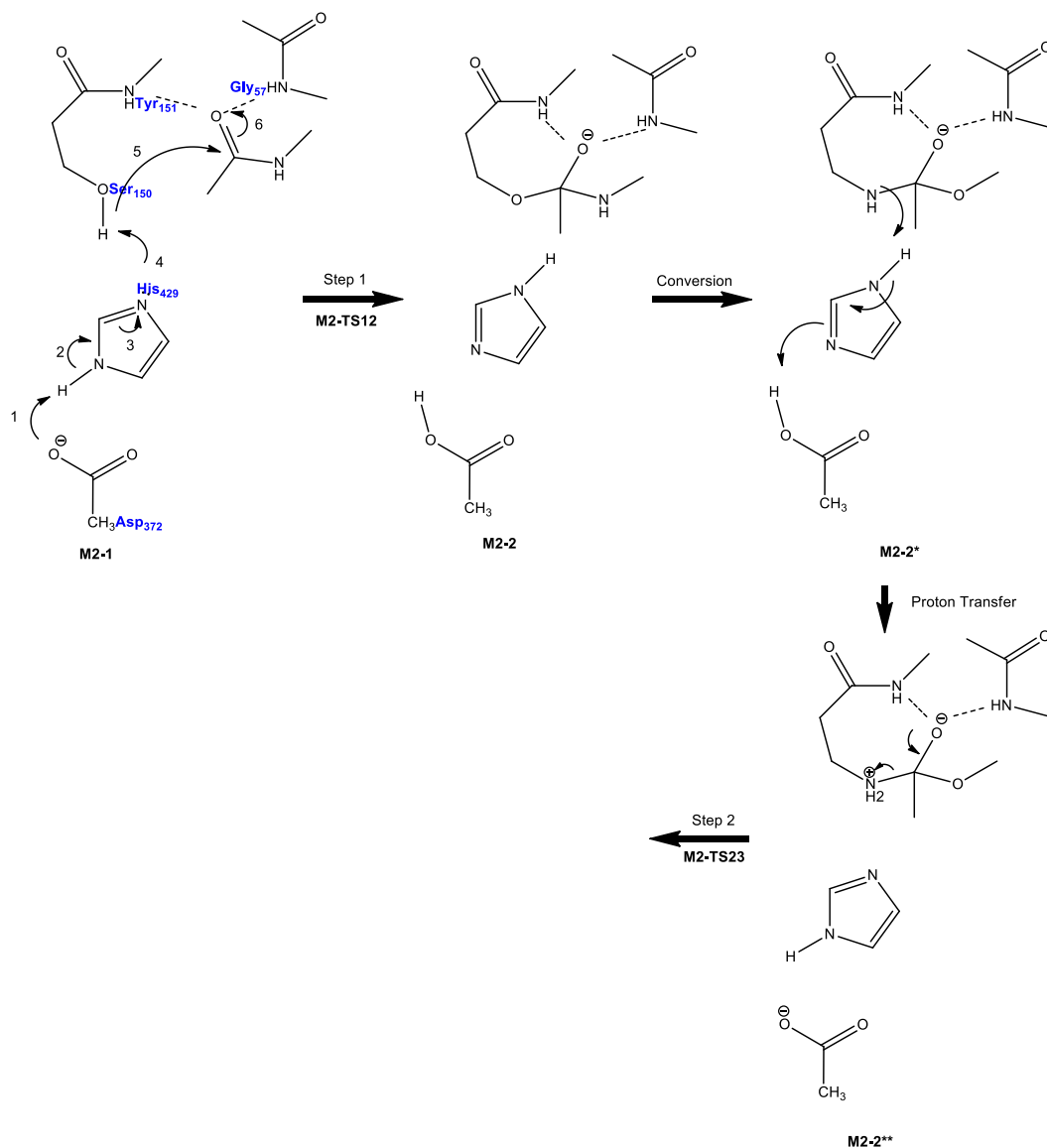
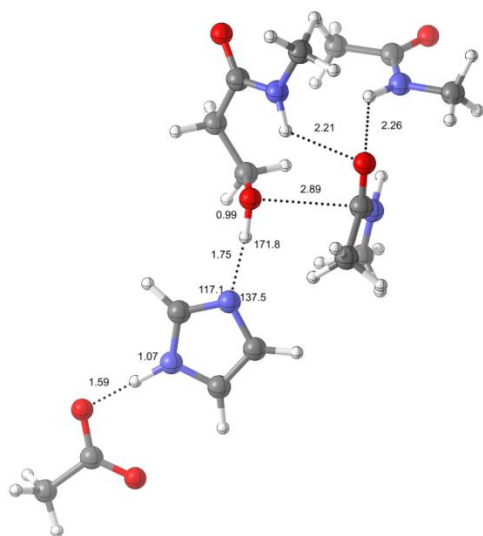
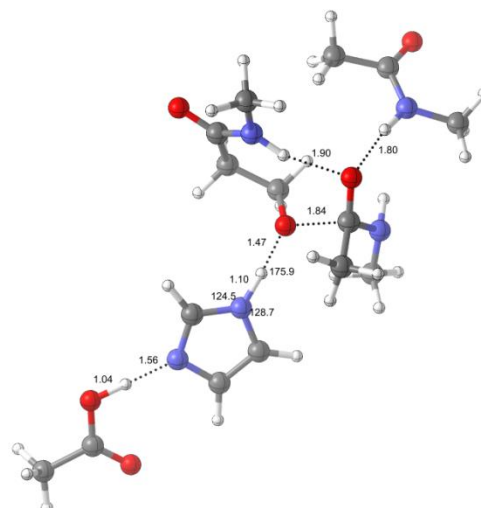


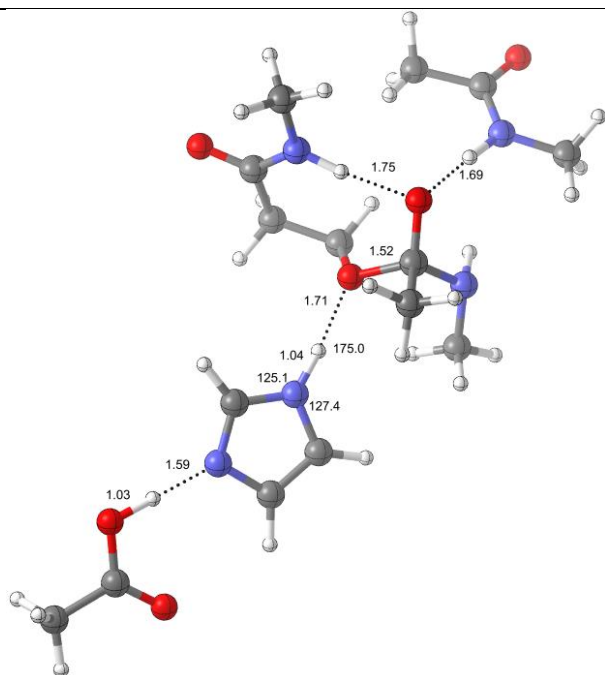
Figure S4: The proposed reaction mechanism of CatA by M2 model study.



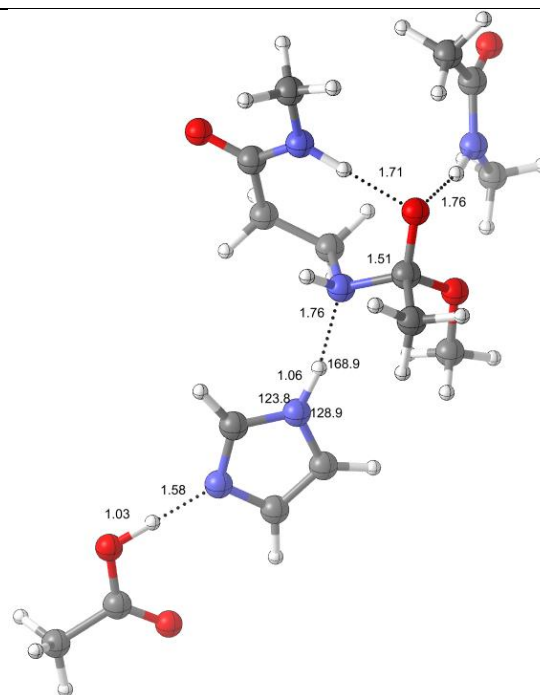
M2-1: 0.00 kcal/mol



M2-TS12: 19.22 kcal/mol



M2-2: 19.02 kcal/mol



M2-2*: 22.82 kcal/mol

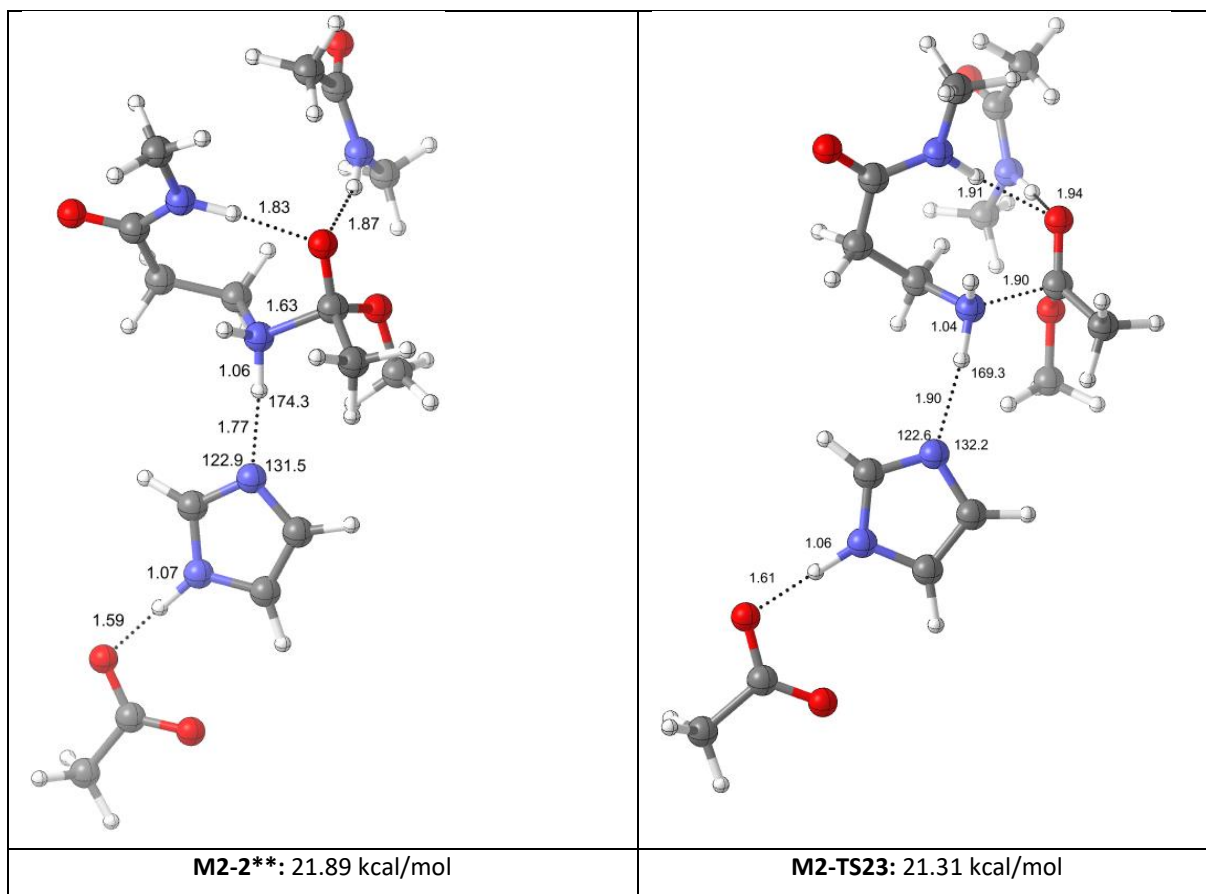


Figure S5. The 3-dimensional geometries (intermediates and transition state structures) of the reaction mechanism of the first model study. (Energies are relative Gibbs Free Energies in kcal/mol)

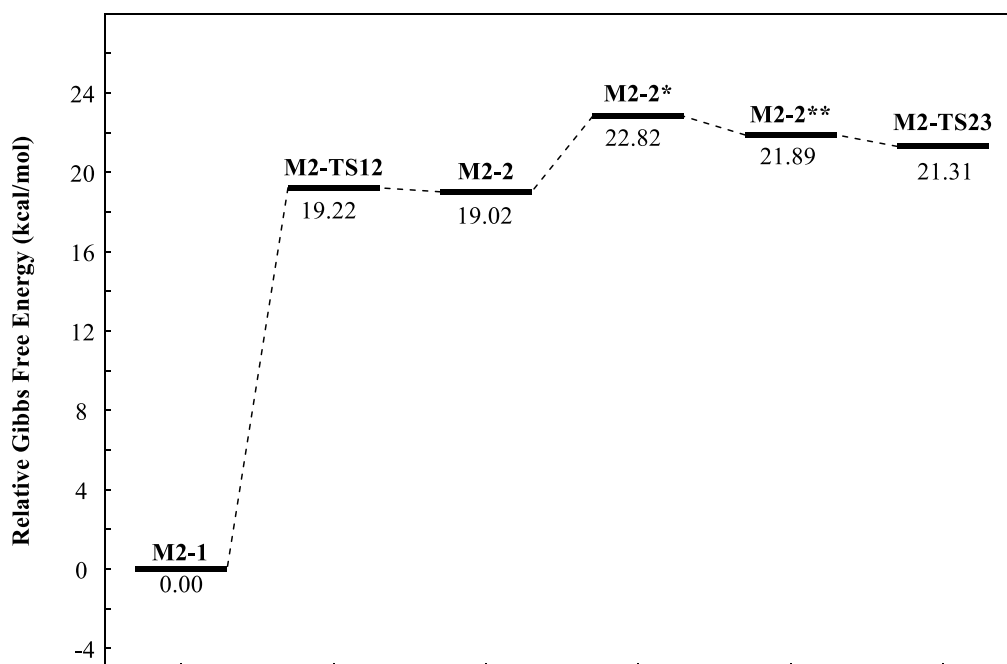


Figure S6. Reaction profile of M2 model study. (Energies are relative Gibbs Free Energies in kcal/mol).

S3. Discussion on CPY, CPW, CatA Difference and Novelty of Asp64 in CatA : Asp64 is substituted by threonine in CPY and tyrosine in CPW (both EC 3.4.16.5 along with CatA). Those enzymes have similar pH activity with CatA but inhibition characteristics of these enzymes along with CatA are different.¹ The effect of Asp64 and this proton transfer was not considered as a topic of our research as well as characteristic differences of CatA, CPY and CPW. However, the situation of Asp64 is examined to discuss potentially important aspects. There are many possible interaction points around Asp64. Thr68 and Met430 side chains are two of those interaction points. In some of the crystal structures, there are crystal waters in the vicinity: When the active site crystal structures are aligned, possible crystal waters' locations from 2 sides of Asp64 are observed. At one site H₂O-768 for 6wia structure and H₂O-2060 for 4cia crystal structure are observed. For the other site; H₂O-2057 for 4az0, H₂O-2220 for 4cib, H₂O-718 for 6wia are located. Last of the interactions is the well discussed Glu69. When Asp64 PROPKA values are compared with Glu69 PROPKA values, it is mostly seen that Glu69 is more acidic than Asp64. 2 structures: 4ci9, an apoenzyme and 6wia, a DFP aged enzyme with an acetic acid/acetate docked to carboxylate binding site are exceptions (see Table S1). In our 2-proton structures starting with **PS2-B** and **PS2-C**'s optimized protonation patterns and the structures in their reaction mechanisms (system **2** for **PS2-B** and system **2'** for **PS2-C**) and related mechanisms, it is observed that deprotonated Glu69 strongly hydrogen bonds Asp64. In the system **2**, the Asp64 proton which was between Glu69 and Asp64, optimized to be closer to Glu69 (a proton transfer from Asp64 to Glu69 is observed). As proton transfer is a probability between Glu69 and Glu149 in the mechanism, there may be conformations which cause a proton transfer or sharing between Asp64 and Glu69. The Asp64's capability of transferring a proton is a novelty for CatA, with respect to CPY and CPW and possible benefits of this capability are in the dark. Khavrutski reported D64N mutant of CatA is insoluble, unlike E69Q and E149Q and E69Q+ E149Q mutants which suggest Asp64 has an effect on solubility of enzyme.² A possible reason could be it's effect on pI of the enzyme so Asp64 could be anionic. When the active site of crystal structures are aligned, the side chain conformations of Asp64 show relatively larger deviation from each other with respect to Glu69 and Glu149 side chains (**Figure S8**). There is somewhat of a cavity around carboxylate group of Asp64 and there are many interaction sites without a strong binding. These suggest Asp64 side chain seems rather flexible.

S4. Discussion on proton transfer between Asp372 and His429

A possible proton transfer between Asp372 and His429 was also investigated with the cluster model. In the model study M2, the proton is moving back and forth between Asp372 and His429 throughout the path, indicating a low barrier hydrogen bond and two-proton transfer mechanism. Also, first intermediates of **4**, **3**, **2**, **2'** systems (**4-2**, **3-2**, **2-2** and **2'-2**) were designed according to M2 model in which Asp372 is protonated and His429 H δ is bonded to Asp372 carboxylate instead of His429. All

clusters were initially designed as $\text{O}\delta_{\text{Asp372}}\text{-H}\delta$ distance as 0.98 Å and $\text{H}\delta\text{-N}\delta_{\text{His429}}$ distance as 1.71 Å. After optimization, these distances were optimized to 1.66 Å and 1.06 Å in **4-2** cluster, to 1.72 Å and 1.05 Å in **3-2** cluster, to 1.77 Å and 1.04 Å in **2-2** cluster and to 1.94 Å and 1.03 Å in **2'-2** cluster, respectively. After all, it was observed that the two proton transfer mechanism is not favored and the hydrogen always prefers binding with His429 during the 1st step of the reaction, a result in comply with NMR and neutron diffraction studies for another serine protease, trypsin³, and the PROPKA results for CatA (see pKa values of Asp372 and His429 at **Table S1**). Results proposed that the low barrier hydrogen bond (LBHB) discussed in the literature does not exist between His429 and Asp372.^{4,5} One other aspect observed in our calculations is that the proton moves from Asp372 to His429 as the negative charge around substrate's carboxylate side (in basic media) gets condensed from **4-2**, then **3-2**, then **2-2** and finally to **2'-2**.

S5. Discussion on Amino Acid Specificity of CatA and Cationic Scissle Aminoacid Selection Over Anionic Aminoacids

Despite CatA is defined as serine carboxypeptidase with broad C-end specificity (**EC 3.4.16.5**), amino acids other than the C-terminal amino acid alter the activity.⁶ The broad specificity term for this enzyme is mostly attributed to glycine, hydrophobic and cationic amino acids of the peptide. On the hydrophobic part, working on dipeptide substrates, Hiraiwa found that hydrophobic/hydrophobic dipeptides showed the highest activity for CatA and CPY.^{7,8} For cationic amino acids and Gly, Jackman's results propose His, Arg and Gly can be cleaved.⁶ In another study, Pshezhetsky researched activity of CatA Phe-X dipeptide derivatives.⁹ The results were interesting. While non-polar amino acids showed most activity, rates of hydrolysis were still considerable amount for Gly and Arg amino acids. More interesting result was the result with the Glu amino acid which showed activity below detection level. These results could lead to a hypothesis which could be supported by our DFT results presented herein: Electron density in the C-end recognition site is somewhat concentrated so that any other anionic side chain would make the reaction harder while with cationic side-chains reaction is easier. This hypothesis can be contradicted by Hiraiwa's results, however.^{7,8} Despite minor activities, Hiraiwa reports Ala-Glu dipeptide successfully cleaved by chicken and bovine CatA.

S6. Discussion on the state of hydrolized peptides in step 3 and step 4 of the catalytic reaction:

During the course of the reaction, the geometrical changes of the carboxylic acid/carboxylate groups and the other atoms of the hydrolyzed amino acid from intermediate-2 (**4-2**, **3-2** and **2-2**) to water complexed intermediates (**4-3W**, **3-3W** and **2-3W**) are not dramatic while there is a general pattern of moving away of the hydrolyzed amino acid from the Ser150/His429 reaction site as the reaction proceeds. In the second step, the cleavage of the peptide bond removes the geometric restriction

while in the following structure, insertion of water causes repulsion between the cleaved amino acid and the Ser/His active site.

The interaction distances of the carboxylic acid/carboxylate group of substrate to the carboxylate binding site of the enzyme (Gly56-NH, Asn55-NH₂, Glu149 /Glu149-H) do not show significant changes in **4**, **3** and **2** systems till water complexed structures. Consequently, it can be deduced that a hydrogen bond network is present between the substrate carboxylic acid/carboxylate and the enzyme during steps 3 and 4 of the reaction, while water makes a nucleophilic attack and the enzyme regenerates. After step 4, the shortened substrate C end COOH may transfer its proton to the hydrolyzed amino acid's NH₂ to deprotonate the C-end of the shortened substrate (thus, activating it for being able to complex with C-end binding site of CatA for the next possible carboxypeptidase reaction from the shortened substrate) and neutralize the hydrolyzed amino acid into its zwitterionic form. This neutralization of hydrolyzed amino acid may enable the hydrolyzed amino acid to leave the binding site easier. It has been demonstrated in a previous study that the consecutive carboxypeptidase activity of CatA is observed for Substance P, amidated Substance P, Eleodisin and Angiotensin I.⁶ It is therefore recommended that a mechanism for this process be established. The concept of "consecutive carboxypeptidase activity" is further discussed on option 1 of 3 proton mechanism further. The approach of "hydrolyzed amino acid staying on C-end binding site until after step 4" is a different approach from that of Khavrutski who naturally proposes the cleaved amino acid (P1') should leave before a water molecule should approach to initiate the step 3 of the reaction². The suggestion is based on a logical basis, that the water should approach the substrate from the point where the C end of the original substrate was located. Thus, there should not be a substrate at the C-end recognition site, removing a stable interaction from the system. This may be the case if His429/Ser150 site is inaccessible by a water molecule from other directions. However, there is currently insufficient evidence to support this hypothesis, especially in the context of small substrates that will not block water. However, the Bouknight's 2020 paper where diisopropyl fluorophosphate inhibited CatA is examined, hints other possibilities:¹⁰ The crystal structure therein (pdb:6WIA) resembles the intermediate-4 structures (**4-4**, **3-4** and **2-4**), in this study, in terms of geometry and concept but the Ser150 oxygen is bound to a P rather than the substrate C as in this study. Additionally, the carboxylate binding site is occupied by the amino acid (glycine) in our case and by acetic acid/acetate in Bouknight's case. Bouknight's structure alone does not prove that water can approach to intermediate-3 (**4-3**, **3-3** and **2-3**) structure from other directions, but, it proposes that the carboxylate binding site is not necessarily required to be vacant in order a water oxygen to be present in the relevant side of the substrate. In activated (excision peptide removed) enzyme structures (pdb codes: 4az0 and 4az3¹¹, 4ci9 4cia and 4cib¹², 4mws and 4mwt¹³, 6wia¹⁰) His429/Ser150 is relatively accessible from the gorge opening of the enzyme. The approach applied

in our study proposes that water can initially travel from other directions to His429/Ser150, thus, the carboxylate binding site interaction can prevail.

S7. The Geometrical Parameters of Transition States and Intermediates From Cluster Calculations

The **2'-2** exhibited distinctive geometrical parameters, indicating that the His429 and its ϵ proton undergoes a rotation towards the carboxylate binding site. A similar trend was also evident in their corresponding **TS12** geometries. For **4**, **3** and **2** systems; the $N_{\text{His}}\text{-}H_{\text{Ser}}\text{-}O_{\text{Ser}}$ angle was calculated as $173^\circ\text{-}177^\circ$ (in comply with the **M1** and **M2** model studies angles that were around $176^\circ\text{-}177^\circ$) in their first transition state structures (**TS12**) (**Table S2**). In the **2'-TS12**, this angle was reduced to 140° , which represents a deviation from the respective linearity of the **TS12**. Additionally, the $H_{\text{Ser}}\text{-}O_{\text{Ser}}$ distance was increased from 1.47-1.55 Å to 1.76 Å. Moreover, the distance between H_{Ser} and the carboxylate oxygen of substrate towards the Glu149 site reduced from 3.60-3.77 Å to 2.30 Å, possibly indicating an electrostatic attraction from C-end binding site in **TS12** in **2'** system. A His429 rotational transition state from “substrate’s carboxylate group interacting structure” to “substrate’s amide nitrogen’s lone pair interacting structure” was designed (**2'-HisRot**) and the barrier to this conformational change was found to be 1.09 kcal/mol higher than the energy of the **2'-2** structure. The structure of **2'-HisRot** is included in **Cartesian Coordinates of the Cluster Structures**.

S8. Deamidase-esterase activity of CatA enzyme

It is known from the literature that deamidase/esterase (neutral substrates), reaction is favored at high pH and de-activated at low pH.^{6,10,12-22} It could be very helpful to cover carboxypeptidase activity and deamidase/esterase activity in calculations with one substrate. However, no such substrate can have a carboxylate end and an amidated/esterified end at the same time, thus this research is limited to carboxypeptidase reaction. The mechanistic insights gained from the calculations herein on carboxypeptidase activity can provide valuable information on the deamidase/esterase activity of CatA as well. At high pH, electron density is considered to be accumulated on carboxylate binding site of the enzyme due to lack of proton and it causes repulsion of the substrate. Such a repulsion could be somewhat hindering neutral amide/ester substrates to approach further into C end binding site of enzyme, thus, keeping the substrate at His429/Ser150 binding site. The nature of the carboxylate binding site (possible proton orientations and their respective enzymatic conformations, probable in-enzyme proton transfers such as 3-proton option 1, 2 and 3 mechanisms discussed earlier (**Figures 11-13**)) makes discussion more complex if they are applied to the deamidase/esterase system. It is seen that the enzyme is able to show carboxypeptidase activity for amidated Substance P and Neurokinin A (which is also amidated). For these substrates, however,

deamidase activity is only observed at high pH.⁶ For Eleodisin (still deamidated) in the same paper showed deamidase activity in both low pH and high pH conditions. It is unclear if carboxylate binding site has some affinity to simple amide $R(C=O)NH_2$ to promote carboxypeptidase reaction over deamidase reaction for amidated substrates. In 1ivy structure, both CatA chains contain a crystal water in place of the C-end binding site. Bouknight revealed that the carboxylate binding site is an interaction site for even a very simple acetic acid/acetate (protonation state arguable) group. Nakase's study further extends the discussion on this topic.²³ Nakase found carboxypeptidase/deamidase preference of amidated substrates and enzyme-substrate interaction extend over S1 and S1' interaction sites. Nakase reported that CPY acted as carboxypeptidase to Fmoc-Glu-Glu-Glu-Glu-Ala-NH₂ substrate and acted as deamidase on Fmoc-Glu-Glu-Glu-Ala-NH₂ substrate.²³ This research lacks qualitative/quantitative data to dictate a preference or comparison of carboxypeptidase and deamidase/esterase reactions, as well as the qualitative/quantitative data on deamidase/esterase reaction's high pH preference over low pH preference. However, it is favorable to highlight and discuss the H-bonding characteristics of these relevant amide and ester substrates with the Glu149 as H-bonding is important at the C-end binding site: Amide and ester groups' carbonyl oxygen are likely to be oriented to Asn55-NH₂ and Gly56-NH because those two hydrogens create an enzyme environment like the oxyanion hole, enabling a sole oxygen to fit in the pocket. The ester group's ester oxygen (likely to be at Glu149 side) has H-bond acceptor capability while it lacks H-bond donor property. The amide N (supposed to be at Glu149 side) is inverse of that- NH₂ can be a proton donor to Glu149 but it can hardly accept protons as the nitrogen lone pair is in conjugation. For these reasons, similar pH activity profile of amide substrate and ester substrate can not be attributed to H-bonding capabilities of substrates. It is already discussed that at high pH Glu69 is deprotonated and Glu149-H is facing towards Glu69 to support anionic structure. This makes only amide to be able to support a proton to Glu149. If the interaction is sufficiently strong, the amide NH₂ group may engage with the carboxylate binding site at high pH, thereby favoring the carboxypeptidase reaction while disfavoring the deamidase pathway. This behavior contrasts with the general trend typically observed. This suggests that at high pH, the C-terminal binding site exerts electronic repulsion towards neutral groups such as amides and esters—likely even more strongly toward the negatively charged carboxylate groups, as observed in the **2'** set of our calculations. An exception to this trend may be the COOH group, which contains a labile proton; this possibility was addressed under Option 1 in the proposed activation/deactivation mechanisms involving the triply protonated ES complex.

Table S1: PROPKA values of various CatA structures.

PROPKA	pH	Asp64	Glu69	Glu149	Asp372	His429
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1ivyA	8.0	7.33	5.74	13.46	4.07	7.11
1ivyB	8.0	7.53	5.96	13.50	3.88	7.25
4az0*	7.4	9.40	6.28	16.62	4.23	10.40
4az3*	7.4	10.34	6.41	16.80	4.19	10.51
4ci9	4.6	6.50	7.67	16.17	3.89	10.48
4cia***	4.6	8.18	5.66	14.18	3.98	6.95
4cib*	4.6	9.14	5.73	14.92	2.59	11.17
4mwsA	7.0	7.28	5.80	13.11	4.00	7.49
4mwsB	7.0	7.29	5.84	13.11	3.99	7.47
4mwtA	7.0	7.30	5.81	13.16	4.03	7.48
4mwtB	7.0	7.31	5.72	13.16	4.02	7.47
6wia**	7.4	6.89	8.53	16.23	4.02	16.92

* ligand docked.

** DFP inhibited and acetic acid bonded as ligand.

*** ligand bonded but ligand not docked to carboxylate binding site

Table S2: Important bond lengths and angles for transition state **N-TS12** and the intermediate **M-2** for all 4 systems studied.

	4		3		2		2'	
	4-TS12	4-2	3-TS12	3-2	2-TS12	2-2	2'-TS12	2'-2
N _{His} -H-O _{Ser}	177	114	174	111	173	110	140	95
H-O _{Ser}	1.55	2.34	1.47	2.40	1.51	2.40	1.76	3.22
N _{His} -H-N _{Subs}		170		168		167		116
H-N _{Subs}		1.76		1.71		1.68		2.41
H-O _{Subs}	3.77	2.55	3.68	2.47	3.60	2.44	2.30	1.56

Table S3: The cutting scheme and the residues involved in the Cluster Model

Residue	Atoms in Model	Frozen Atoms
TRP 53	Only side chain	C β
LEU 54	C α , C, O	C α
ASN 55	Whole	-----

GLY 56	Whole	H of NH
GLY 57	N, C α	C α
SER 61	C α , C, O, Side chain	C α
SER 62	Whole	-----
LEU 63	N, C α , C, O	-----
ASP 64	Whole	-----
GLY 65	Whole	-----
LEU 66	N, C α , C, O	-----
LEU 67	N, C α , C, O	-----
THR 68	N, C α , C, O	-----
GLU 69	Whole	-----
HIS 70	N, C α , Side chain	C α
GLY 148	C α , C, O	C α
GLU 149	Whole	-----
SER 150	Whole	-----
TYR 151	N, C α , C β , C, O	-----
ALA 152	Whole	-----
GLY 153	N, C α	C α
VAL 176	C α , C, O	C α
GLY 177	Whole	-----
ASN 178	Whole	-----
GLY 179	Whole	-----
LEU 180	N, C α	C α
VAL 371	C α , C, O	C α
ASP 372	Whole	-----
MET 373	N, C α , C β , C, O	-----
ALA 374	Whole	-----
CYS 375	Whole	-----
ASN 376	N, C α	C α
GLY 428	C α , C, O	C α
HIS 429	Whole	-----
MET 430	N, C α , Side chain	C α

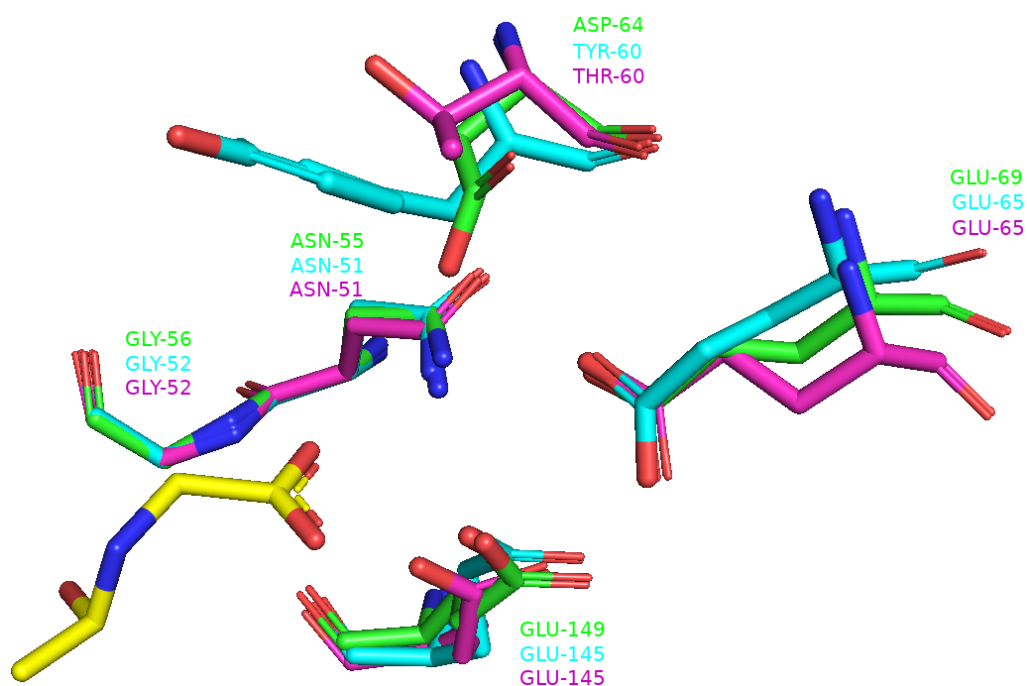


Figure S7. Carboxylate binding site alpha carbon aligned crystal structures of CatA (4cia green) CPY (1ysc purple) and CPW (1whs cyan) with a representative ligand (yellow)

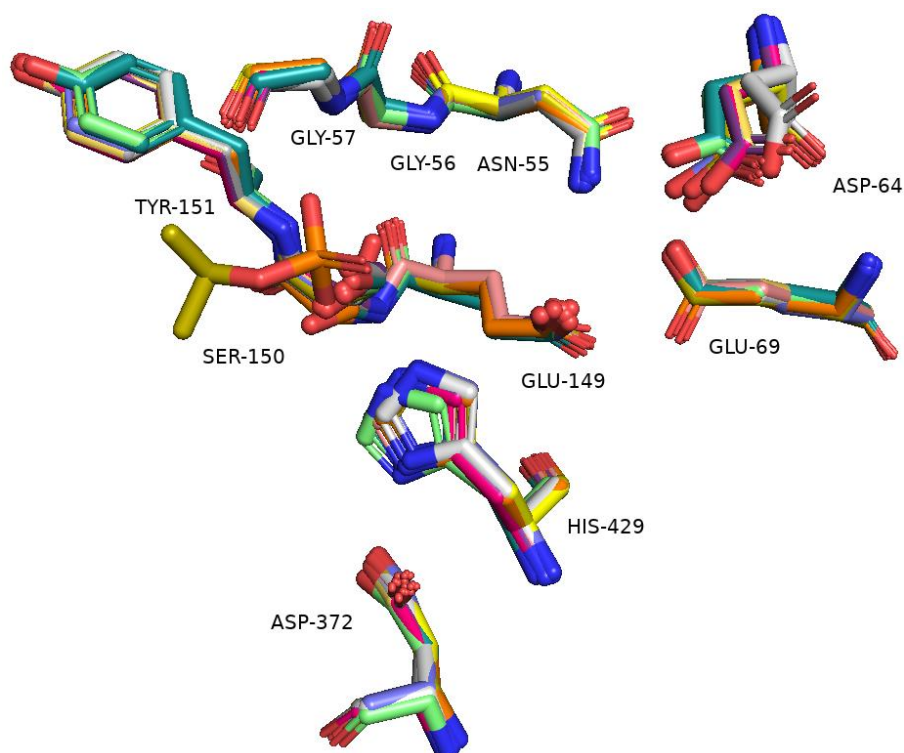


Figure S8. Active sites' alpha carbon aligned for all active site CatA crystal structures in the literature (1ivy chainA and ChainB light green and dark green, 4az0 shiny yellow, 4az3 pale rose, 4ci9 pale grey, 4cia blue, 4cib orange, 4mws chain A shiny pink, 4mws chain B pale yellow, 4mwt chain A purple, 4mwt chain B grey, 6wia dark yellow)

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Cartesian Coordinates of the Cluster Structures

4-1

Grid = Ultrafine

No negative frequency

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4-TS12

Grid = Ultrafine

1 negative frequency (TS) at -239.89 cm^{-1} , Intensity = 26.50 km/mol

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4-2

Grid = Ultrafine

No negative frequency

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4-TS23

Grid = Ultrafine

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4-TS34

Grid = Ultrafine

1 negative frequency (TS) at -679.65 cm^{-1} , Intensity = 4336.91 km/mol

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4-4

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H -4.352072 6.707546 -0.997198
H -5.664772 4.659744 -2.003651

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4-TS41

Grid = Ultrafine

1 negative frequency (TS) at -402.20 cm^{-1} , Intensity = 2312.99 km/mol

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4-1*

Grid = Ultrafine

No negative frequency

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3-1

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3-TS12

Grid = Ultrafine

1 negative frequency (TS) at -231.35 cm^{-1} , Intensity = 116.81 km/mol

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3-2

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3-TS23

Grid = Ultrafine

1 negative frequency (TS) at -1026.05 cm^{-1} , Intensity = 5312.84 km/mol

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Grid = Ultrafine

No negative frequency

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3-3W

Grid = Ultrafine

No negative frequency

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3-TS34

Grid = Ultrafine

1 negative frequency (TS) at -740.75 cm^{-1} , Intensity = 4746.10 km/mol

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3-4

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3-TS41

Grid = Ultrafine

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2-1

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C -5.320436 6.511025 1.031745
O -5.953399 5.822084 1.829512
H -5.079417 8.320290 2.115442

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2-TS12

Grid = Ultrafine, loose optimization criteria

2 negative frequencies, TS one is at -28.49 cm^{-1} , Intensity = 18.88 km/mol

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H -4.413421 -2.615280 -5.687696
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2-2

Grid = Ultrafine

No negative frequency

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2-TS23

Grid = Ultrafine

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2-3

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2-TS34

Grid = Ultrafine

1 negative frequency (TS) at -432.77 cm^{-1} , Intensity = 1466.22 km/mol

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2-1*

Grid = Ultrafine

No negative frequency

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2'-1

Grid = Ultrafine

No negative frequency

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2'-TS12

Grid = Ultrafine

1 negative frequency (TS) at -53.79 cm^{-1} , Intensity = 17.07 km/mol

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2'-HisRot

Grid = Ultrafine

1 negative frequency (TS) at -54.26 cm^{-1} , Intensity = 20.19 km/mol

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2'-TS23

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2'-3pre

Grid = Ultrafine

No negative frequency

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2'-TS23-2

Grid = Ultrafine

1 negative frequency (TS) at -64.34 cm^{-1} , Intensity = 58.82 km/mol

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