

Supplementary Data

Table S1 Average Binding Energy and its Components Obtained from the MM-GBSA Calculation for the complex

MM-GBSA	ΔE_{vdw}	ΔE_{ele}	ΔG_{polar}	$\Delta G_{\text{nonpolar}}$	ΔG_{total}
	-62.84±6.23	-140.30±21.77	190.58±19.27	-11.62±0.79	-24.18±5.92

Table S2 Binding energy and its components of key residues

Residue	ΔE_{vdw}	ΔE_{ele}	ΔG_{polar}	$\Delta G_{\text{nonpolar}}$	ΔG_{total}
ASN84	0.2965	-3.1678	1.2319	-0.0701	-1.7095
THR85	-0.5293	0.5934	-0.5462	-0.0005	-0.4826
PRO86	-3.8054	-1.9612	1.8743	-0.5482	-4.4405
GLY87	-1.3069	-1.0802	1.1456	-0.1029	-1.3444
TYR88	-0.2625	-0.1332	0.212	-0.0006	-0.1843
SER89	-0.3867	-1.0197	1.2547	-0.1045	-0.2563
TYR97	-3.0746	-0.2836	1.2382	-0.4914	-2.6113
GLY154	-0.0319	-0.0072	-0.1764	0	-0.2155
MET155	-0.9664	-0.8337	0.291	-0.046	-1.5552
SER156	-1.0177	-1.1814	1.4453	-0.1718	-0.9256
GLY158	-0.0523	-0.2072	0.0661	0	-0.1935
TRP197	-0.1759	0.4168	-0.5449	-0.0047	-0.3087

ILE200	-1.1424	-0.0048	0.0041	-0.2712	-1.4143
TYR390	-0.9825	-0.1923	0.9932	-0.2047	-0.3863
GLU391	-1.0626	-8.7716	8.5871	-0.4094	-1.6564
THR392	-1.9668	-1.9991	2.4646	-0.1554	-1.6567
ALA393	-2.1521	-1.818	1.958	-0.4675	-2.4795
GLN394	-0.8574	-2.8423	2.9183	-0.2748	-1.0562
TYR396	-0.2975	-0.1062	0.3122	-0.0169	-0.1085
SER432	-1.0985	-0.5683	1.8381	-0.3213	-0.15
LYS433	-1.8658	2.1092	-0.7608	-0.3484	-0.8658
ASN434	-0.4918	-0.4205	0.7635	-0.1077	-0.2565
PHE438	-0.2062	-0.0284	0.1417	-0.0725	-0.1655
GLN445	-0.7043	-0.4355	0.939	-0.1402	-0.341
GLY446	-0.2096	0.1592	-0.1443	-0.0316	-0.2263
GLU447	0.6079	-20.7081	16.7905	-0.3654	-3.6751
GLN531	-0.1697	-0.2375	0.2147	-0.0006	-0.193
ASP533	1.9391	-25.0192	18.592	-0.425	-4.913
HIE565	-2.6153	-0.6375	1.3067	-0.5222	-2.4683
THR566	-1.3792	-0.161	0.4575	-0.1836	-1.2663

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10      20      30      40      50
TanLp   DADLVPEQVQVAGQAIYYAARNIQYVQHPVA.AIQVNVFVPAAYLHGSS.....
TanAs1  NSKWKYD.....SKNNVYQLNLSYVSNPQAKNVEKLGIVYVPAAYFKGKKNHNGYTV
TanLb   STANQYN.....AEDDVYQIGISYVCEPDDTSVETLAVFVPGAYMTAADNGDGYTC
TanAsg  INQWIFD.....ETNNCYMSLKNVYCAQPKDSELEALHIFVPAAYMTADGTDIDR...
TanBFnn NPDKYVSKETEINGQKIKYRAYENIVYVKNPIDKDYONNNIYIPEEFVFNSS.....
TanBlpe DADLVPEQVQVAGQAIYYAARNIQYVQHPVA.AIQVNVFVPAAYLHGSS.....
TanBlpa DADLVPEQVQVAGQAIYYAARNIQYVQHPVA.AIQVNVFVPAAYLHGSS.....

60      70      80      90      100     110
TanLp   .....VNGYQRAITAPITMNPNTVGGYLPGPDDPQRVTWPTNAGTIQQAQKRQYVVVA
TanAs1  TVNDAKKVNQYARITAPITMNPNTVGGYLPGPDDPQRVTWPTNAGTIQQAQKRQYVVVA
TanLb   EINTEGSLGSYADTAPITMNPNTVGGYLPGPDDPQRVTWPTNAGTIQQAQKRQYVVVA
TanAsg  AVVINKNGTITVTSQVPIFYNDIGGYAECQPAVMT.....PRNQRVLEDGVVLSV
TanBFnn .....IGSYVSSNAPITMNPNTVGGYLPGPDDPQRVTWPTNAGTIQQAQKRQYVVVA
TanBlpe .....VNGYTRDTAPITMNPNTVGGYLPGPDDPQRVTWPTNAGTIQQAQKRQYVVVA
TanBlpa .....VNGYQRAITAPITMNPNTVGGYLPGPDDPQRVTWPTNAGTIQQAQKRQYVVVA

120     130     140     150     160
TanLp   GTRGRITVDDK.....SGQRVQAPAFIVDMKAAHRYVKYNQGRLPGDANRRIITNGSA
TanAs1  GTRGRSMSGMGNSSNASTSYETIGSFWGIVTDKAAHRYVRFNDSLPGNSKRIYTFGSSG
TanLb   GCRGRD.....SGAFAGVTDKAAHRYIRYTDVLPGDAESITFGMSG
TanAsg  GARGRQSQ.....NGIGKAPAGLVDDKAAHRYLRLKHHNDIPGDIETKISVNGSA
TanBFnn GARGRITLDN.....KGNITGKAPAAIVDDKAAHRYLYLNDVMPGDANKRIITNGSA
TanBlpe GTRGRITVNE.....SGQRVQAPAFIVDMKAAHRYVKYNQGRLPGNVRIITNGSA
TanBlpa GTRGRITVDDK.....SGQRVQAPAFIVDMKAAHRYVKYNQGRLPGDANRRIITNGSA

170     180     190     200     210
TanLp   GGA*SALAGASGNSAYEFEPALTAGAA.P.....ATDDIFAVSAYCBIHNLEHADMAYE
TanAs1  GGA*SALAGASGNSAYEFEPALTAGAA.P.....ATDDIFAVSAYCBIHNLEHADMAYE
TanLb   GGA*SALMGSTGSDLYDAYLEEGAVMG.....VSDAVLGSMCWCBIHNLEHADMAYE
TanAsg  GGA*SALGSGTGNRAEYLSFLEEIGAEELD.....QRDDIFAAQCFBIHNLEHADMAYE
TanBFnn GGA*SALGATGNSSDYLPYKKEIGAAE.....TRDDIFAVSAYCBIHNLEHADMAYE
TanBlpe GGA*SALAGASGNSAYEFEPALTAGAA.P.....ATDDIFAVSAYCBIHNLEHADMAYE
TanBlpa GGA*SALAGASGNSAYEFEPALTAGAA.P.....ATDDIFAVSAYCBIHNLEHADMAYE

220     230     240     250     260     270
TanLp   WQFNGINDMHRYPQVAGITKN...GRPKFEPVSGQLTVEEQATSLALKAQFSTYLNQLK
TanAs1  WQMGQYGNM.....GNRKKNSFQKQLSTDLASSYASVYLNKLN
TanLb   WMGVTRSG.....LSE...EQLSQSLAEAFAMINSAG
TanAsg  WQFQAKKIYTFNSVRPQ.....IINKRQQLSGLAEFPFVYVNSL
TanBFnn WQFNGVNSYSRMEFTRNSAQEYNDRSLTRSTVQGNLTDEIKISNKLTFPFWNSLK
TanBlpe WQFNGINDMHRYPQVAGITKN...GRPKFESTIGLSSADQSSADLKRQFSTYLNQLK
TanBlpa WQFNGINDMHRYPQVAGITAVN...GRPKFEPVSGQLTVEEQATSLALKAQFSTYLNQLK

280     290     300     310     320     330
TanLp   LKNGN.TLISLTKSRNGQVTEGSYAKYIKKETEDSATEFLNNTTFPYKQNSTEQAGMGNG
TanAs1  IKDEDGNVLLISESTEGIYQSGTYDYDKTIVIEESLNNPLSDTFEPYDASSGMMGGFG
TanLb   LDES...LTADGRGNFYQ...GILNQLLSLNLKFLAKHAQTNDE.....
TanAsg  LTTDAGNSLTLDKNGSFK...TYLSIIRNS...ANKALK...
TanBFnn LHDANGCALTVSPDGTGTFQ...NYLVQLLTD...ACALD...
TanBlpe LTAGSDGTHLTLNEAGMGSFR...DVVRLLISS...ACTAFD...
TanBlpa LKATDGTTLVTIAAGTGFPR...EVVRHLMAS...ACTALD...

TanLp   .....
TanAs1  GPS.....G.....GK.....FSGKMGSPQMR...
TanLb   GGMRGGNGGMSFRNGEKPDGERPFGGEGDGPDPGTDGKPDGEGAPSFEEGEMPDMDTTE
TanAsg  .....
TanBFnn  .....
TanBlpe  .....
TanBlpa  .....

340     350
TanLp   .....QGT*DHKYA.GFAVT..GNQVTDLDSAY
TanAs1  .....KQSSNKTYKTDAYLKDINKKRTWITYDKTKRAHITSLIKDF
TanLb   SEQSFEMDDITRNDITGGLSLSGTYETAQDYIDALNTDGEWVIYDASTNTAITSIEDF
TanAsg  .....KEELARELDPQGLWCHFE..NGQATVFDLIDAY
TanBFnn .....EGKDISQFKKAFITIE..NKKVVAVDLDVY
TanBlpe .....KGV*DHKYA.GFTVT..NGRVTGLDLKAY
TanBlpa .....QGT*DHKYA.GFVVT..GNQVTDLDSAY

360     370     380     390     400
TanLp   LK.SLTRMKAVPAFD*LDLITSPENNLFGDATA.KAKHFA*ALAQTRS.....
TanAs1  AKYKQPKS*SVSAFD*DLNRSQAE*EVFGTSGSDSKLHF*OSLAKLLTENKSNYSKINGWN
TanLb   VKAFK*SASKNLGAFD*DLNEGQGENTLFCYGD.GNGAFD*EILSQILTD.....LG
TanAsg  VVNYMGRK*KCPAFD*SLVYQTPETEVF*GNRDK.NHRHF*ENVAKHIEKLPALS.....
TanBFnn TH.IGRMK*SPAFD*SLDASSGENLFG*DKKS.DNKH*FKSFDINNKAIEYFSSGKFN
TanBlpe LT.SLTRMKAVPAFD*LDLGLSLENLFG*DATV.MNRHF*FSQEH.....
TanBlpa LK.SLTRMKAVPAFD*LDLITSPENNLFG*DALV.LGKHFA*ALSQARS.....

410     420     430     440
TanLp   .....IVTAC.....ADAE*LI...QAINP*SYLTTT...SSQVAKHWR*IHHGA*ARD*
TanAs1  SNYVSSYKNDLTKTKLGTSMSTRMNYNPMYLLSDYSGYKSNVANHWR*ITGICQGG*
TanLb   SSYASAYAE*DSQDDAGNTVDVRLAMYTL*YLLLESSEGYETS*VARVWR*ITGICQGG*
TanAsg  .DYQAFQVD...AREDL*LARKL*MPYTLQSD...LEBK*QVASHWR*ITGICQGG*
TanBFnn DKNKISVFK...AKN*IL...KMN*PTLQNN...TSTKYWR*IHHGA*ARD*
TanBlpe .....TATAQL...APEL*V...QAINP*SYLTTG...QSAKNAQWR*IHHGA*ARD*
TanBlpa .....IVTAC.....ADADD*V...KAVN*PSYLLTQ...QAVAKHWR*IHHGA*ARD*

450     460     470     480     490
TanLp   TSFA*PIILATML*LNH...CYGIDFALP*WDIP*SGDYD...LGLFSAW*IDLGL*CQ..
TanAs1  TALNTE*NLSLALKERVGSKNVDFKTVDQCHTMAETSGNSDSNF*IKWVE*SINNK..
TanLb   CALSTE*MNLALALENYSGVEDVDFETVWAGHTQAERTGSSTGN*FIAWNEC*MSEA
TanAsg  TSFA*ISYLLALALKR...GIDVHYELI*WGMHADADY...NEEFSQW*DAI*VHK..
TanBFnn TSLA*IPAILALKL*RMS...GKVDVDFASP*WGC*GGDYD...LELFW*IDLGL*CQ..
TanBlpe TSFA*PIILATML*LNQ...GREVDFALP*WDIP*SGDYD...LGLFSAW*IDLGL*CQ..
TanBlpa TSFA*PIILATML*KNP...CYGIDFALP*WDIP*SGDYD...LGLFSAW*IDLGL*CQ..

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Fig.S1 Multiple sequence alignment of TanA_{Lb} from *Lachnospiraceae* (MBQ6323131.1), TanA_{Lp} from *Lactiplantibacillus plantarum* (BAH20446.1), TanA_{Sl} from *Staphylococcus lugdunensis* (BAF03594.1), TanA_{Sg} from *Streptococcus gallolyticus* UCN34 (YP_003431024.1), TanB_{Fnn} from *Fusobacterium nucleatum subsp. polymorphum* (ALQ42581.1), TanB_{Lpe} from *Lactiplantibacillus pentosus* (BAN10247.1), TanB_{Lp} from *Lactobacillus plantarum* (BAG68453.1) and TanB_{Lpa} from *Lactiplantibacillus paraplantarum* (BAN10246.1). The three conserved catalytic residues Ser, Asp, and His are indicated by green stars.

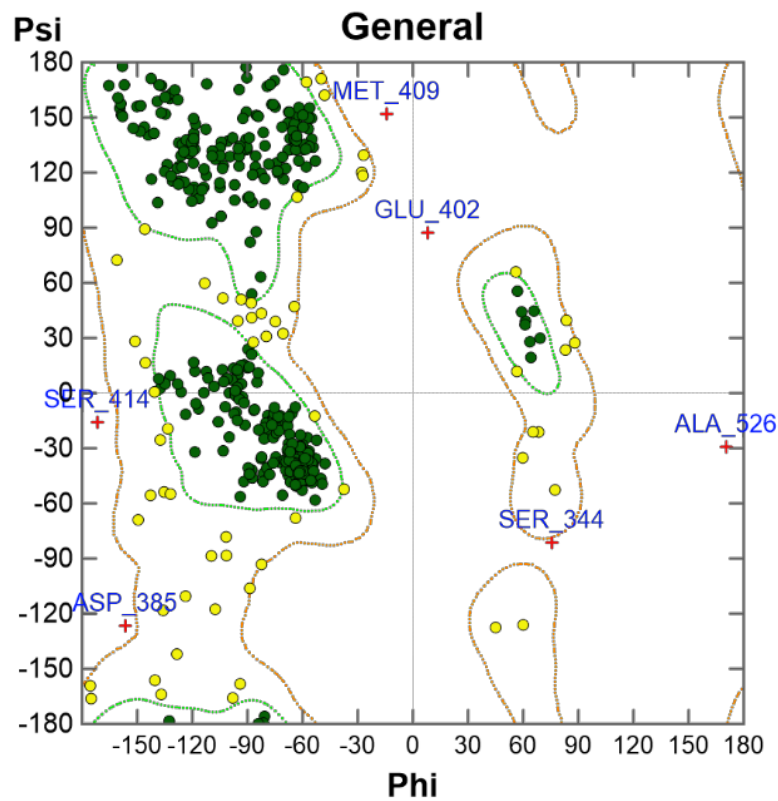


Fig.S2 Ramachandran plot for TanA_{Lb}. Dark green dots represent the residues in favored regions; yellow dots represent the residues in allowed regions, red cross represent the residues in irrational regions.

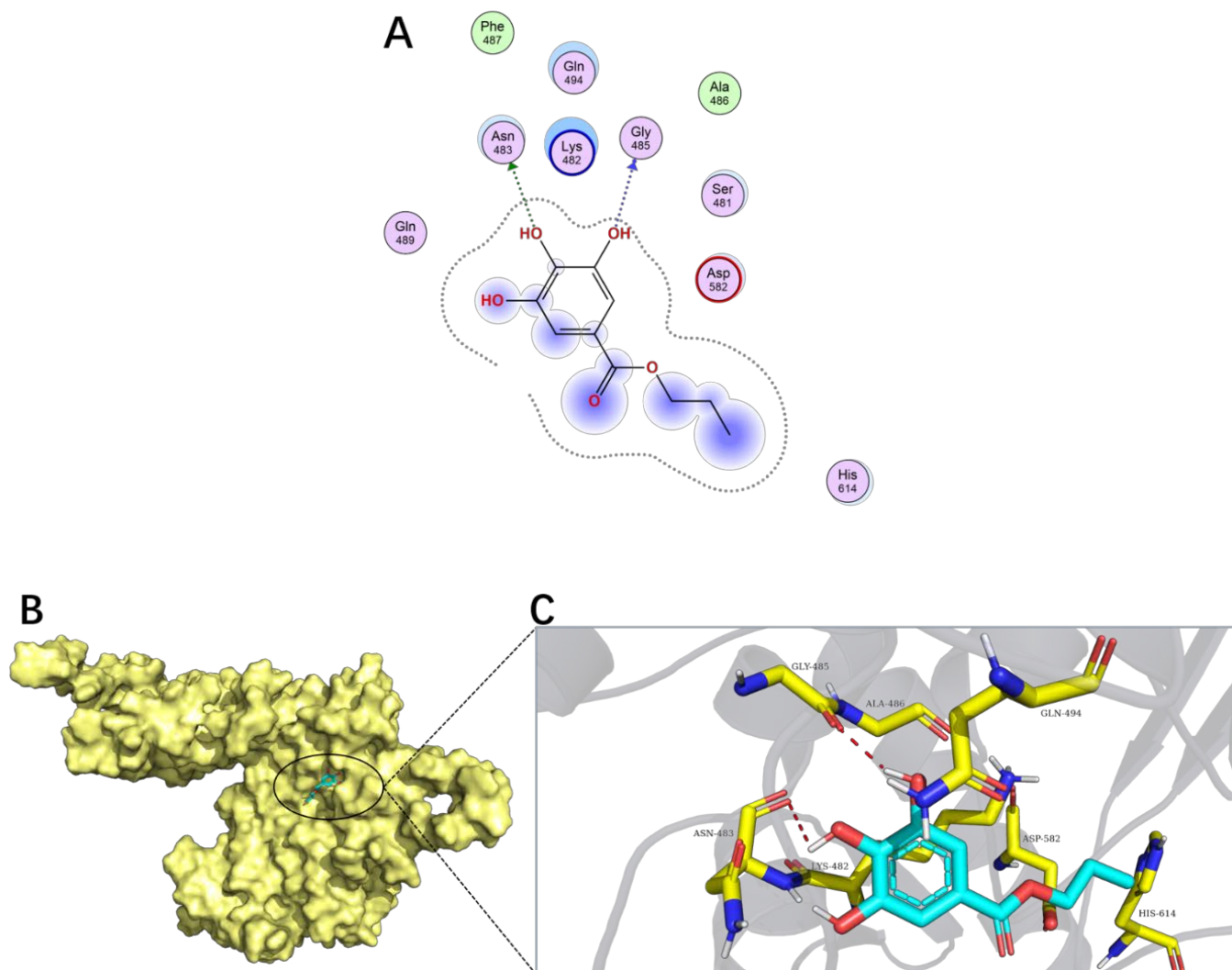


Fig. S3 Complex of TanA_{Lb} and propyl gallate. (A) The 2D binding mode of TanA_{Lb} and propyl gallate. (B) The binding model of propyl gallate on molecular surface of TanA_{Lb}. Propyl gallate is colored in cyan, the molecular surface of tannase is colored in pale yellow. (C) The 3D binding mode of tannase and propyl gallate. Propyl gallate is colored in cyan, the surrounding residues in the binding pockets are colored in yellow, the backbone of the receptor is depicted as white cartoon with transparency.

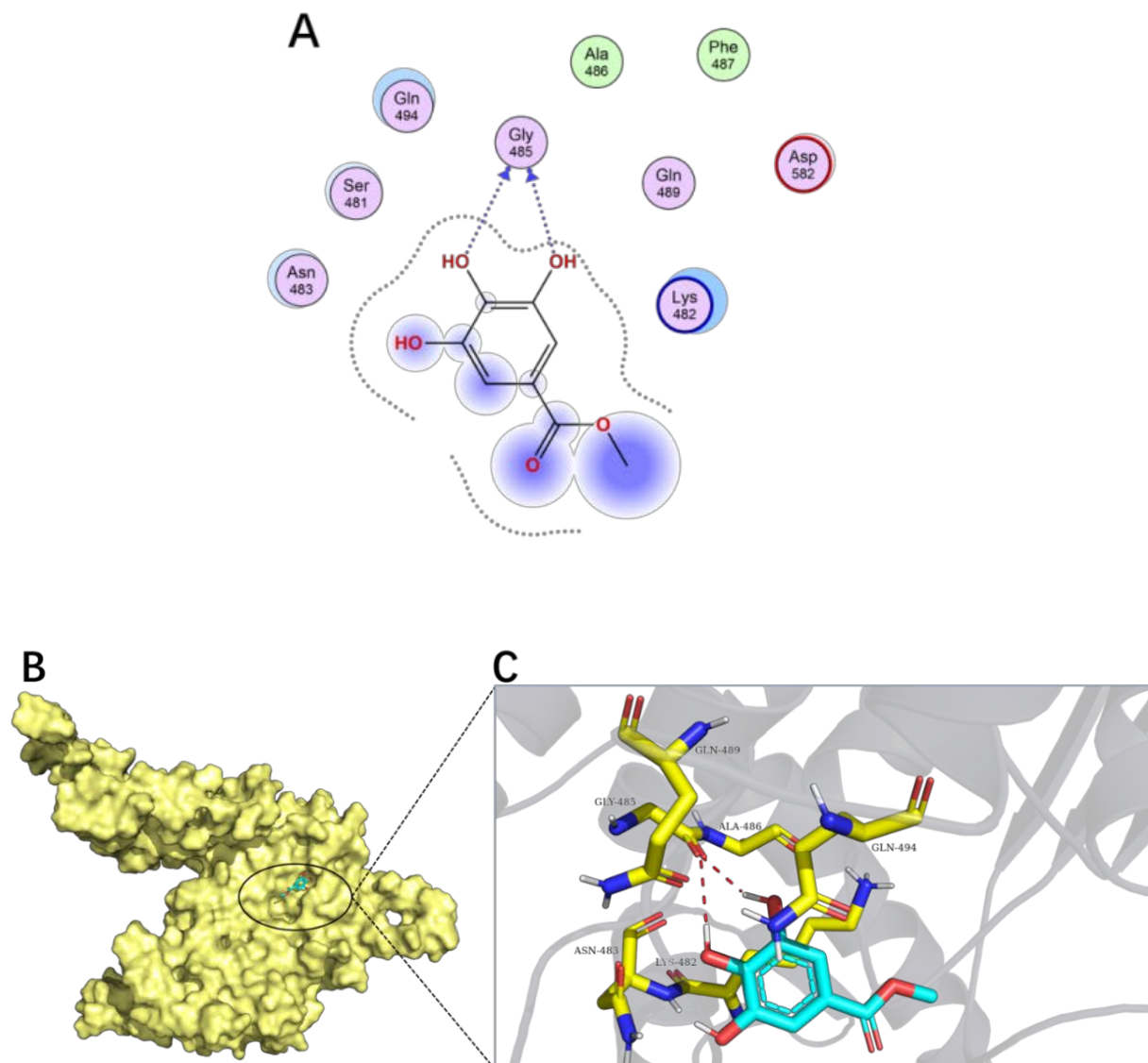


Fig. S4 Complex of TanA_{Lb} and methyl gallate. (A) The 2D binding mode of TanA_{Lb} and methyl gallate. (B) The binding model of methyl gallate on molecular surface of TanA_{Lb}. Methyl gallate is colored in cyan, the molecular surface of TanA_{Lb} is colored in pale yellow. (C) The 3D binding mode of TanA_{Lb} and methyl gallate. Methyl gallate is colored in cyan, the surrounding residues in the binding pockets are colored in yellow, the backbone of the receptor is depicted as white cartoon with transparency.

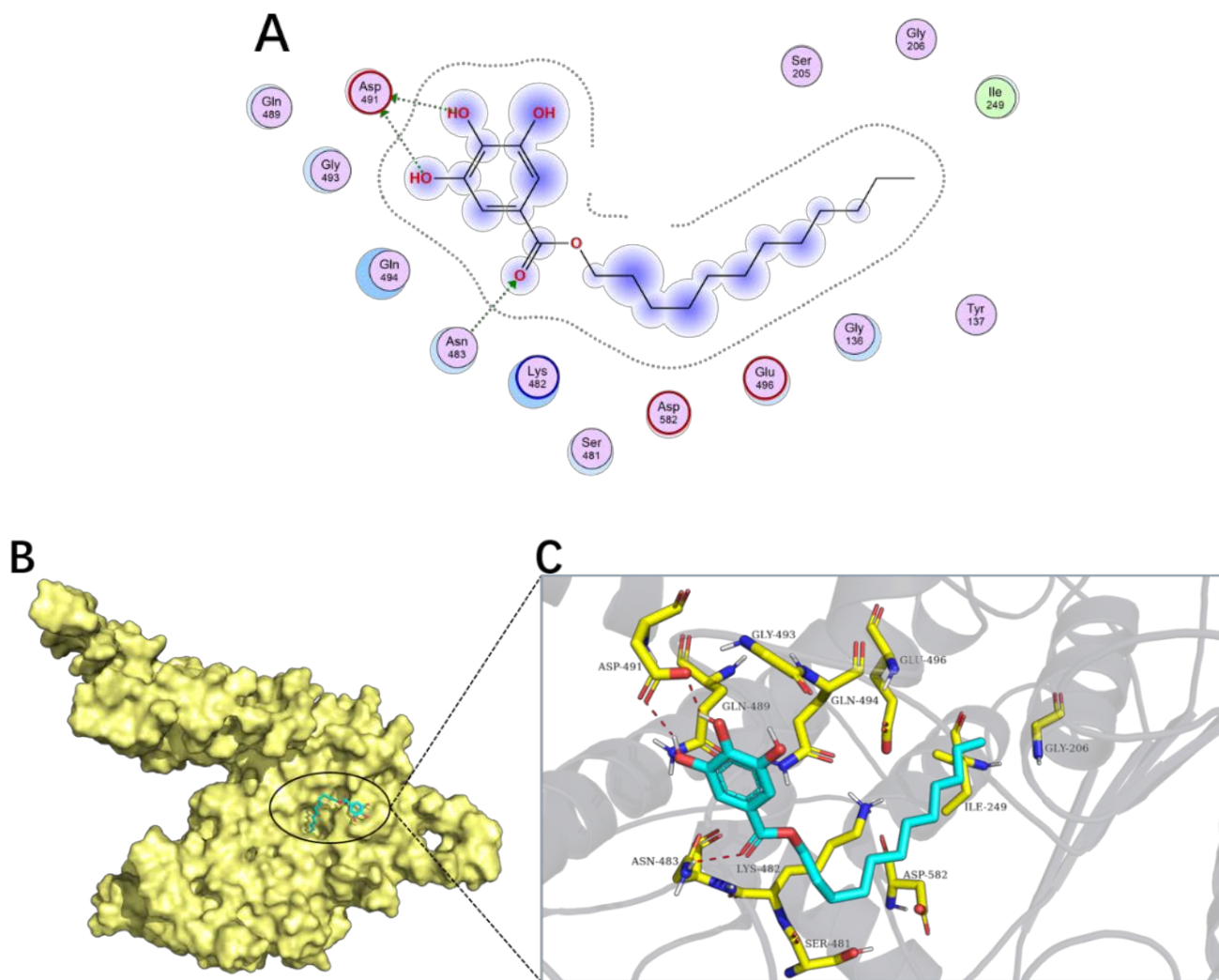


Fig. S5 Complex of TanA_{Lb} and Lauryl gallate. (A) The 2D binding mode of TanA_{Lb} and lauryl gallate. (B) The binding model of lauryl gallate on molecular surface of tannase. Lauryl gallate is colored in cyan, the molecular surface of TanA_{Lb} is colored in pale yellow. (C) The 3D binding mode of TanA_{Lb} and Lauryl gallate. Lauryl gallate is colored in cyan, the surrounding residues in the binding pockets are colored in yellow, the backbone of the receptor is depicted as white cartoon with transparency.

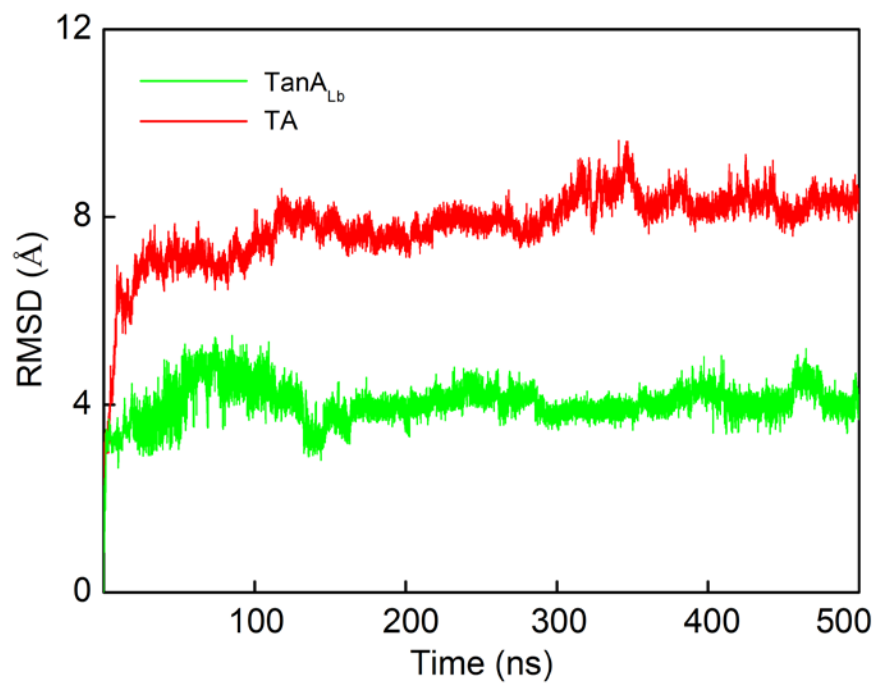


Fig. S6 RMSD of the TanA_{Lb} and tannic acid during the 500ns simulation.