Interactions of small molecules with a degrading enzyme uncovered by quantum mechanics/molecular mechanics (QM/MM) calculation and molecular dynamic (MD) simulation

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Supporting information

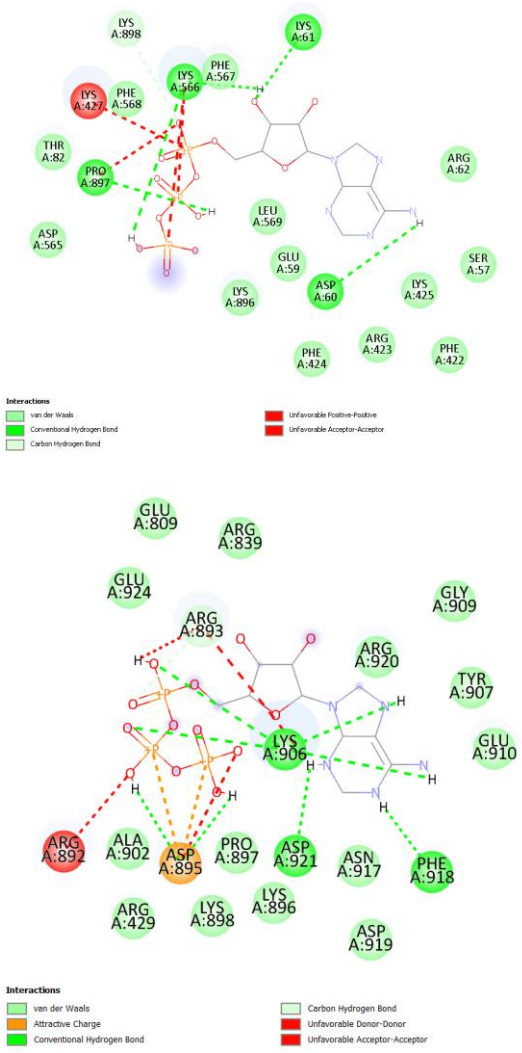

Fig. S1 2D The conformers after QM/MM minimisation using Ambertools20 and CP2K, simulated by Discovery Studio

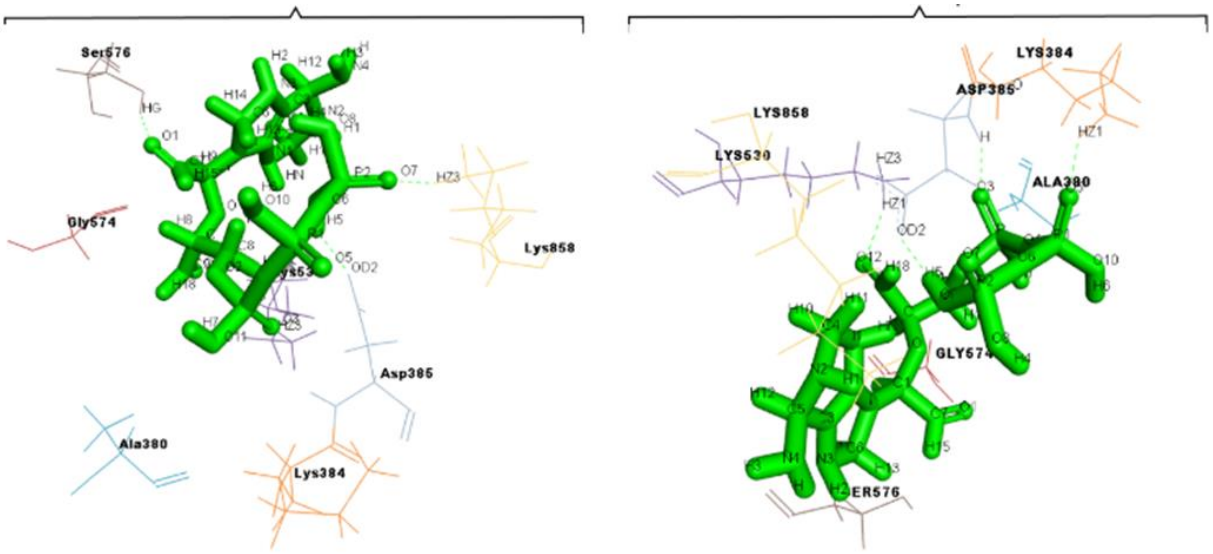

Fig. S2 3D The conformers after QM/MM minimisation using Ambertools20 and CP2K, simulated by Discovery Studio

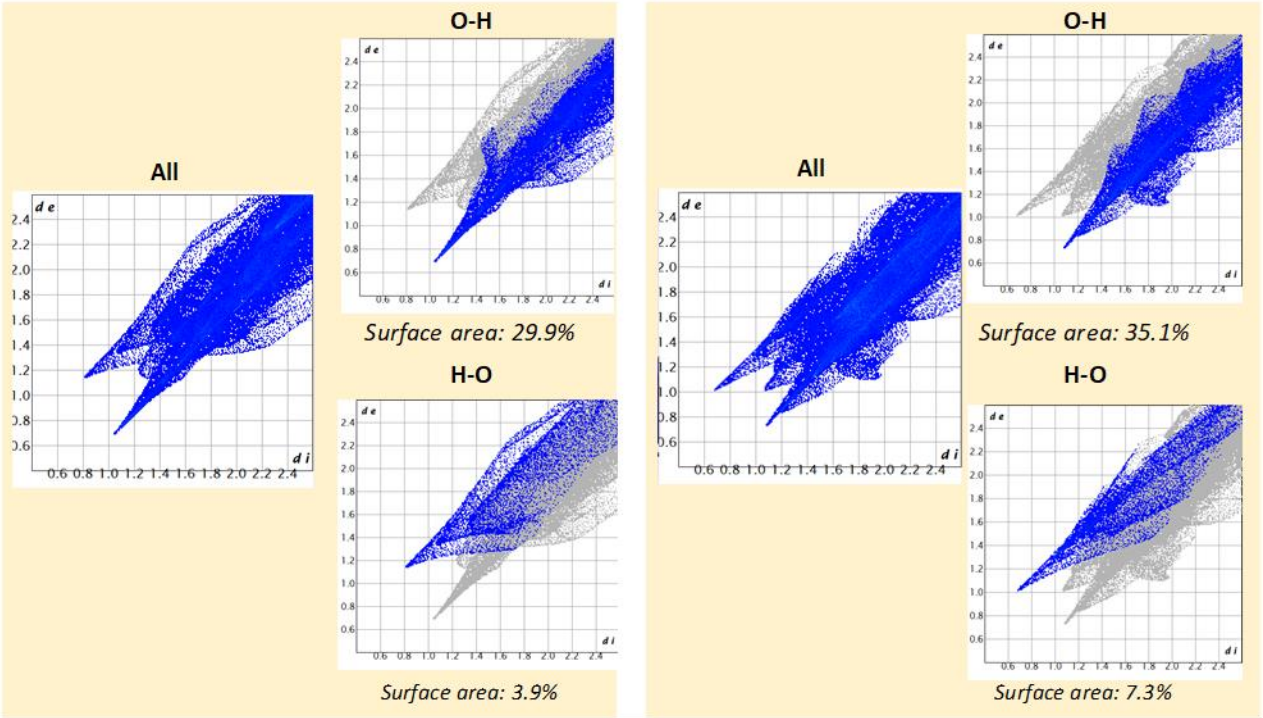

Fig. S3 Surface area of hydrogen bonding interactions, simulated by CrystalExplor

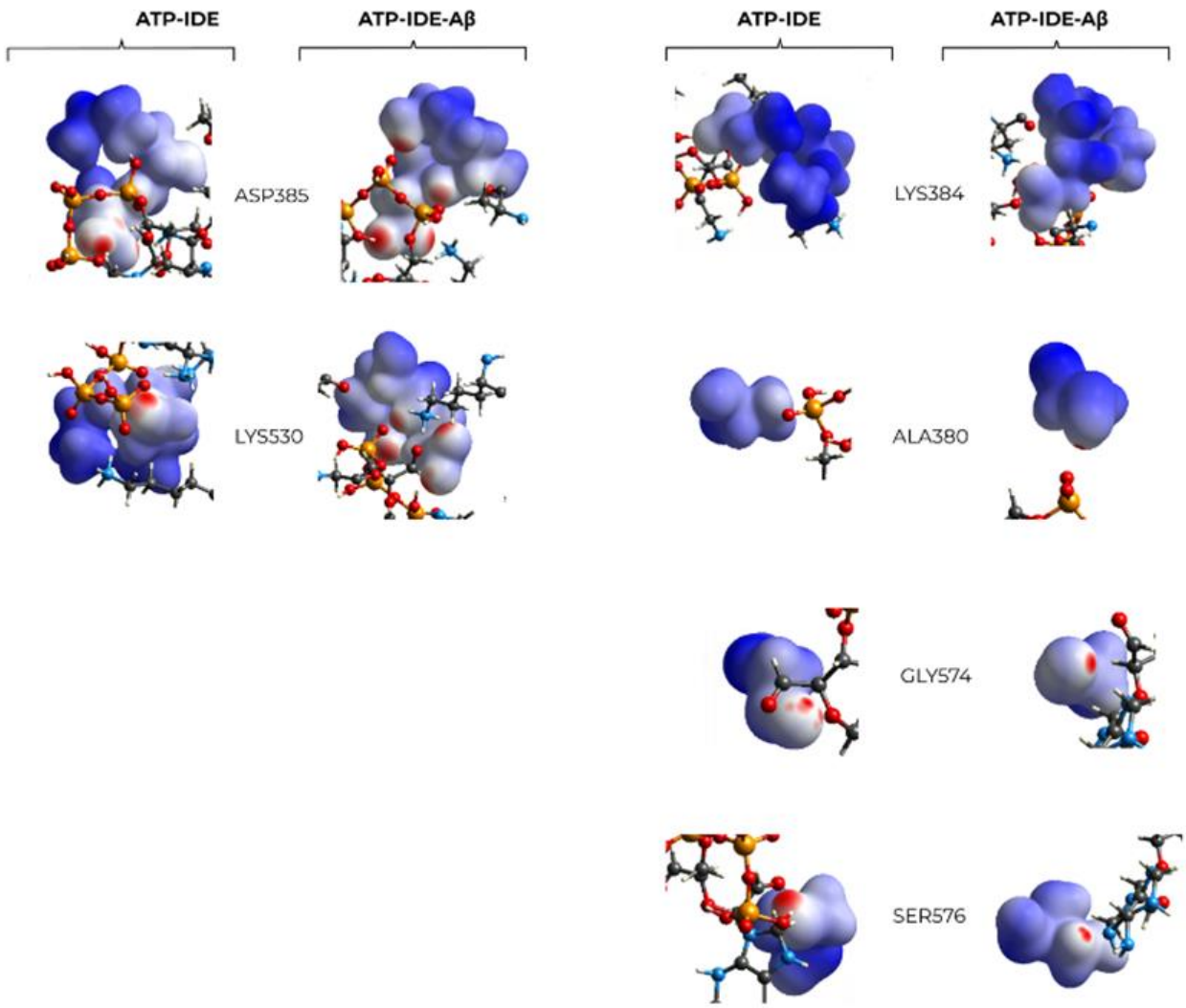

Fig. S4 Normalise contact distance (D_{norm}) map among amino acids of the small molecules and degrading enzymes, based on density functional theory (DFT) calculation, shows the electron density of interactions with proximity. Both systems are shown in the same angle and settings. Red, white and blue colour of 3D surface area indicate closed, medium and little proximity, respectively.

Table S5 Results of molecular mechanic energy minimisation

List	**System 1**	**System 2**
NSTEP	4000	4000
ENERGY	-5.16E+05	-5.15E+05
RMS	2.45E-01	2.46E-01

GMAX	2.52E+01	3.45E+01
BOND	39138.5368	38780.853
ANGLE	2419.0879	2444.7027
DIHED	11373.8595	11483.6963
VDWAALS	94328.1848	92611.8532
EEL	-705821.4977	-703438.135
HBOND	0	0
1-4 VDW	3196.1475	3230.605
1-4 EEL	39542.3983	40303.8859
RESTRAINT	0	0

Table S6 Results of thermalization

List	**System 1**	**System 2**
NSTEP	15000	15000
TIME(PS)	30	30
TEMP(K)	173.52	173.58
PRESS	0	0
Etot	-391932.9285	-391746.167
EKtot	46384.3456	46419.0554
EPtot	-438317.2741	-438165.2224
BOND	1982.2664	2008.1777
ANGLE	5852.8398	5924.5176
DIHED	12251.1086	12380.5189
1-4 NB	3498.171	3525.3691
1-4 EEL	39576.305	40332.1215
VDWAALS	64173.4753	64062.1152
EELEC	-565651.4402	-566398.0425
EHBOND	0	0
RESTRAINT	0	0

Table S7 Results of pressure equilibration

List	**System 1**	**System 2**
NSTEP	15000	15000
TIME(PS)	60	60
TEMP(K)	298.13	298.11
PRESS	-193.1	-190.7
Etot	-311079.6707	-311046.5039
EKtot	79693.7356	79719.4358
EPtot	-390773.4063	-390765.9397
BOND	3022.8091	3054.9166
ANGLE	8295.4115	8402.4885
DIHED	12786.5709	12924.9022

1-4 NB	3663.0759	3706.5283
1-4 EEL	39559.4327	40332.6545
VDWAALS	44992.4569	44888.6567
EELEC	-503093.1634	-504076.0865
EHBOND	0	0
RESTRAINT	0	0
EKCMT	34147.9091	34099.9163
VIRIAL	40086.2248	39968.8972
VOLUME	1398571.153	1394475.518
Density	0.9531	0.9563