digzyme *insilico* DMS

digzyme × ANCAT

What is ANCAT?
It is a platform provided by ANPLAT Inc. that enables you to perform a wide range of data analysis methods without requiring specialized knowledge.

Just 3 easy steps!

❶ Register to use ANCAT
❷ Upload your sequence to the cloud
❸ Receive analysis results within **48 hours!**

Predicts many mutation sites that humans would never think of!

Hit rate: 40%※

※Prediction of kcat for single mutations registered in the public database "BRENDA."

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	digzyme *In silico* DMS	Company A Iterative saturation (ISM)	Company B Library approach	Company C Random
Enzymes that are difficult to extract or assay	◎	✗	✗	✗
Prediction of enzyme activity outside the active site pocket	◎	✗	△	△
Number of mutants	◎	○	△	✗

Prediction results

| mutation	activity predict1 (out of pocket)	activity up probability1	thermostability predict	thermostability up probability	solubility predict	solubility up probability	activity predict2 (in pocket)	activity up probability2	activity ratio3	up prob3
A35V	up	0.67	up	0.71	up	0.69	–	–	down	0.06
A35S	up	0.52	down	0.07	down	0.16	–	–	down	0.08
V30A	up	0.50	down	0.02	down	0.07	–	–	down	0.05
L235T	up	0.43	up	0.74	down	0.41	–	–	stay	0.32
V30I	stay	0.29	down	0.06	up	0.86	–	–	down	0.05
V115A	stay	0.22	up	0.88	up	0.70	–	–	up	0.44
V115L	stay	0.20	down	0.02	up	0.65	–	–	down	0.37
V115M	stay	0.17	down	0.00	down	0.16	–	–	up	0.50
L73F	stay	0.15	up	0.66	up	0.71	–	–	up	0.61
V115I	stay	0.10	down	0.07	up	0.54	–	–	down	0.29
S186A	stay	0.07	down	0.25	down	0.28	–	–	down	0.13
A140P	stay	0.06	down	0.00	down	0.16	–	–	down	0.06
Q175S	stay	0.03	down	0.069	up	0.59	–	–	down	0.23
Q175R	stay	0.02	down	0.07	up	0.67	–	–	down	0.18
A140N	stay	0.02	down	0.02	down	0.17	–	–	down	0.02
Q175D	stay	0.01	down	0.30	up	0.73	–	–	down	0.23
V172I	stay	0.01	down	0.35	down	0.39	–	–	down	0.02
A65S	down	0.18	down	0.30	up	0.85	up	0.50	down	0.03
L210F	down	0.17	up	0.85	up	0.97	down	0.12	down	0.07

Prediction trends

AI can propose unique mutation sites!

Enzyme active site pocket

- The training data includes numerous experimental results of random mutation introduction, which the AI learns from extensively.
- Mutations are proposed not only around the pocket but also at residues distant from it, positions that differ from human empirical rules.
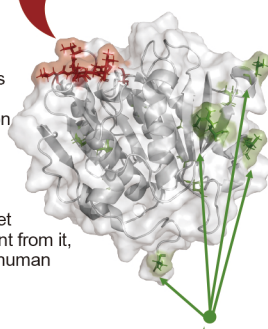
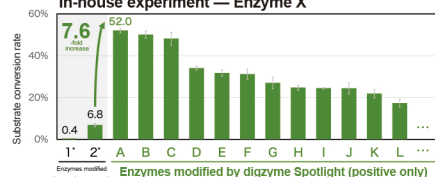**Proposes many residues around the pocket!**

PoC validation

Conducted PoC with 8 companies!

NAGASE
TOYOBO
Green Earth Institute
TOSOH
Other 4 companies!

PoC validation results

Cases	Number of experiments	Number of mutants with improved function
Enzyme A	84	23
Enzyme B	48	21
Enzyme C	9	3
Enzyme D	23	11
Enzyme E	18	2
Enzyme F	28	4
Enzyme G	6	2
Enzyme H	79	51
Enzyme I	71	22
Enzyme J	70	39

Representative case: In-house experiment — Enzyme X

7.6 fold increase
52.0
0.4   6.8
1* 2*
Enzymes modified by previous research
Enzymes modified by digzyme Spotlight (positive only)
Substrate conversion rate

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digzyme, Inc

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