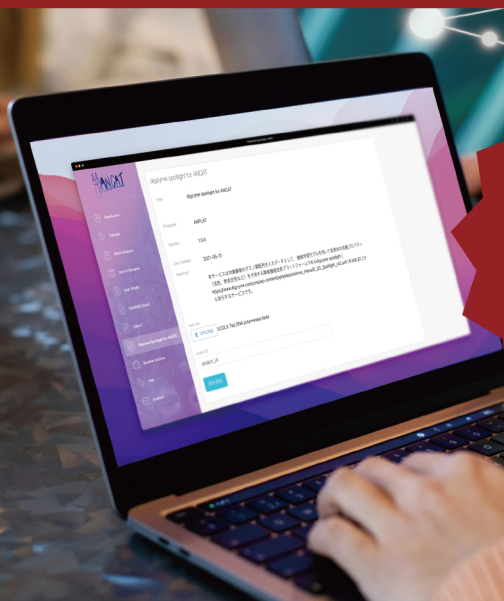# digzyme *insilico* DMS

digzyme × ANCAT

? What is ANCAT?
ANCAT is a platform by ANPLAT that enables any data analysis without specialized knowledge

Just 3 easy steps!

❶ **Register to use ANCAT**

❷ **Upload sequence to the cloud**

❸ **R&D results in 48hrs!**

Predicts many mutation sites beyond human intuition

Hit rate: 40% ※

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

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digzyme **In silico DMS**

	digzyme In silico DMS	Company A Iterative saturation (ISM)	Company B Library approach	Company C Random
Analysis of enzymes difficult to extract or assay	◎	✕	✕	✕
Prediction of enzyme activity outside the pocket	◎	✕	△	△
Number of mutants	◎	○	△	✕

Prediction results

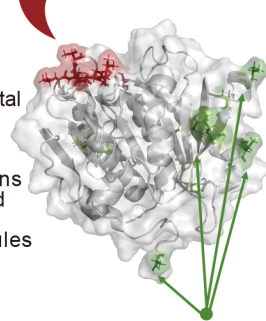| mutation	activity predict1 (out of pocket)	activity up probablity 1	thermostablity predict	thermostablity up probability	solubility predict	solubility up probability	activity predict2 (in pocket)	activity up probablity2	activity ratio3	up prob3
A35V	up	0.67	up	0.71	up	0.69	–	–	down	0.06
A35S	up	0.52	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	–	–	up	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	up	0.25	down	0.28	–	–	down	0.13
A140P	stay	0.06	down	0.00	down	0.16	–	–	down	0.09
Q175S	stay	0.03	up	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	up	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 AI extensively learns from experimental results of random mutations.
- It proposes mutations near the pocket and at distant residues, beyond empirical rules

Proposes many residues around the pocket!

PoC validation

Conducted PoC with 8 companies!
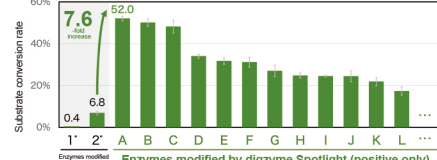
NAGASE
TOYOBO
Green Earth Institute
TOSOH
Other 4 companies!

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

A B C D E F G H I J K L — Enzymes modified by digzyme Spotlight (positive only)

Substrate conversion rate

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digzyme, Inc

SUMITOMO FUDOSAN TORANOMON TOWER 6F, Room 4
2-2-1 Toranomon, Minato-ku, Tokyo, 105-0001, Japan

Official Website

Contact Form

Linkedin