Supplementary Information for:

Deep learning redesign of PETase for practical PET degrading applications

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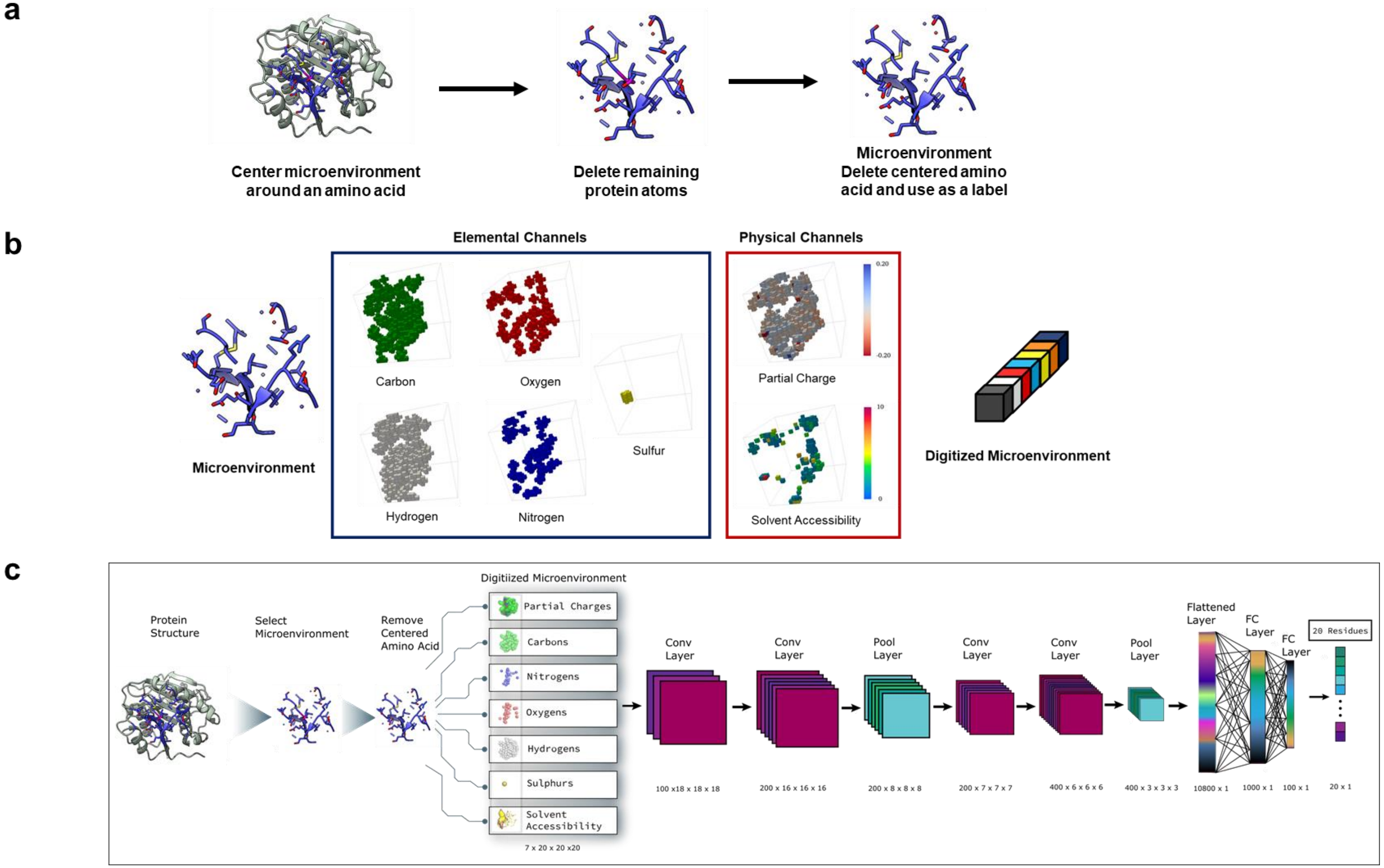


Supplementary Information Fig. 1 | Schematic diagram of Mutcompute. a. Creating a microenvironment: MutCompute begins by centering itself on the alpha carbon of a particular residue in the protein and filters all peptide atoms within a 20 angstrom cube (the orientation of the cube is normalized with respect to the protein backbone). In the filtering process, we create an artificial, self-supervised label by excluding all atoms that belong the center residue. **b.** Encoding the microenvironment: The filtered atoms are then encoded into a 7-channel voxelated representation with a voxel resolution of $1A^3$. **c.** Running MutCompute on a Microenvironment: The 7-channel voxelated representation of a microenvironment is then passed to the CNN model, MutCompute. The model can be broken into 2 parts: Feature extraction and classification. The feature extraction portion consist of convolutional and max pooling layers and is then flattened into a 1D-vector before being passed to the classification layers of the model. The output is a probability mass function of the likelihood each of the 20 amino acids was the amino acid in the center of the microenvironment. We do this process for every residue in the protein to identify residues for mutagenesis.

				Probability distribution across all 20 amino acids																			
pdb_id	**pos**	**wtAA**	**wt_prob**	**ALA**	**ARG**	**ASN**	**ASP**	**CYS**	**GLN**	**GLU**	**GLY**	**HIS**	**ILE**	**LEU**	**LYS**	**MET**	**PHE**	**PRO**	**SER**	**THR**	**TRP**	**TYR**	**VAL**
6ij6	233	ASN	0.09%	1.E-05	1.E-02	9.E-04	2.E-04	2.E-05	5.E-03	4.E-03	3.E-07	6.E-04	1.E-03	5.E-04	1.E+00	4.E-04	2.E-04	1.E-06	8.E-05	3.E-04	2.E-05	1.E-04	9.E-04
6ij6	91	GLN	0.09%	9.E-06	6.E-05	6.E-05	9.E-07	3.E-05	9.E-04	3.E-05	6.E-08	2.E-07	1.E+00	4.E-05	2.E-04	1.E-04	3.E-09	2.E-07	2.E-05	6.E-03	1.E-08	1.E-08	1.E-02
6ij6	225	ASN	0.32%	3.E-04	9.E-06	3.E-03	7.E-07	1.E+00	2.E-05	9.E-07	4.E-07	4.E-07	1.E-05	1.E-04	3.E-07	1.E-04	3.E-08	2.E-07	2.E-04	2.E-02	4.E-09	2.E-09	1.E-03
5xjh	140	THR	0.41%	7.E-05	2.E-06	1.E-02	1.E+00	2.E-03	3.E-05	6.E-04	5.E-07	2.E-06	5.E-07	1.E-05	1.E-05	3.E-06	1.E-07	1.E-07	1.E-02	4.E-03	9.E-08	2.E-07	2.E-05
6ij6	61	SER	0.54%	4.E-04	9.E-04	3.E-02	2.E-01	2.E-03	1.E-02	9.E-02	9.E-06	9.E-03	2.E-02	2.E-02	1.E-03	1.E-03	1.E-03	2.E-05	5.E-03	3.E-01	2.E-04	2.E-03	3.E-01
5xjh	121	SER	0.70%	2.E-03	2.E-02	3.E-02	4.E-02	2.E-03	1.E-01	5.E-01	3.E-05	7.E-03	5.E-04	2.E-03	2.E-01	2.E-03	2.E-04	1.E-03	7.E-03	6.E-04	2.E-05	1.E-04	7.E-04
5xjh	58	SER	0.81%	4.E-03	2.E-02	3.E-02	1.E-01	1.E-03	6.E-02	5.E-01	9.E-05	3.E-03	7.E-03	8.E-02	1.E-01	2.E-03	5.E-04	4.E-05	8.E-03	4.E-03	1.E-04	3.E-04	7.E-03
5xjh	95	LYS	1.06%	2.E-04	8.E-04	1.E-02	2.E-02	2.E-03	2.E-01	6.E-01	2.E-07	2.E-05	4.E-02	1.E-03	1.E-02	2.E-03	9.E-07	5.E-07	9.E-03	4.E-03	4.E-07	9.E-07	1.E-01
5xjh	279	THR	1.98%	9.E-03	2.E-02	1.E-01	5.E-01	2.E-03	3.E-02	2.E-01	2.E-04	9.E-03	5.E-03	3.E-03	3.E-02	2.E-03	1.E-03	1.E-04	8.E-02	2.E-02	2.E-04	8.E-04	9.E-03
5xjh	263	ASP	2.25%	7.E-05	2.E-05	5.E-02	2.E-02	4.E-04	5.E-02	8.E-03	9.E-07	9.E-01	7.E-07	2.E-05	5.E-04	6.E-03	2.E-04	2.E-07	9.E-05	1.E-04	2.E-06	5.E-04	6.E-07
6ij6	58	SER	2.30%	8.E-01	1.E-02	6.E-03	3.E-02	4.E-04	8.E-03	1.E-01	1.E-03	4.E-04	2.E-04	6.E-03	2.E-02	6.E-04	1.E-04	5.E-05	2.E-02	4.E-03	4.E-05	2.E-04	3.E-03
6ij6	53	ARG	2.82%	1.E-04	3.E-02	1.E-02	4.E-04	7.E-05	3.E-01	7.E-02	1.E-06	3.E-05	3.E-04	7.E-03	6.E-01	8.E-03	5.E-06	1.E-06	2.E-04	1.E-04	5.E-06	6.E-06	2.E-04
6ij6	34	ARG	2.99%	4.E-07	3.E-02	2.E-02	2.E-04	8.E-05	3.E-03	5.E-04	3.E-07	1.E-01	3.E-02	8.E-01	2.E-02	4.E-03	6.E-04	6.E-07	2.E-05	1.E-03	4.E-05	9.E-05	5.E-04
6ij6	208	ILE	3.02%	4.E-04	4.E-03	4.E-04	3.E-04	3.E-04	6.E-04	8.E-04	3.E-06	7.E-05	3.E-02	5.E-04	1.E-03	5.E-04	3.E-05	1.E-05	6.E-04	7.E-02	1.E-05	1.E-05	9.E-01
6ij6	59	ARG	3.25%	2.E-02	3.E-02	6.E-02	5.E-02	6.E-03	6.E-02	1.E-01	3.E-04	3.E-03	4.E-03	1.E-03	9.E-02	3.E-03	4.E-04	2.E-04	2.E-01	3.E-01	5.E-05	5.E-04	6.E-02
6ij6	224	ARG	3.52%	1.E-05	4.E-02	1.E-02	3.E-04	1.E-05	4.E-01	1.E-02	4.E-07	3.E-03	6.E-06	2.E-01	4.E-01	1.E-02	1.E-03	5.E-07	8.E-06	3.E-06	2.E-03	1.E-03	5.E-07
5xjh	262	MET	3.74%	5.E-06	8.E-06	1.E-02	9.E-05	2.E-03	3.E-04	9.E-05	5.E-07	3.E-05	2.E-01	7.E-01	5.E-05	4.E-02	3.E-06	8.E-07	7.E-06	6.E-04	3.E-07	5.E-07	5.E-02
6ij6	136	SER	4.15%	2.E-02	3.E-05	7.E-03	1.E-01	2.E-02	5.E-03	4.E-02	7.E-05	2.E-03	1.E-04	6.E-04	2.E-04	5.E-04	4.E-04	1.E-05	4.E-02	7.E-01	2.E-05	2.E-04	9.E-02
5xjh	233	ASN	4.51%	6.E-04	3.E-03	5.E-02	7.E-03	5.E-04	2.E-02	1.E-02	1.E-06	7.E-02	2.E-05	3.E-04	8.E-01	4.E-04	1.E-03	7.E-07	2.E-03	1.E-03	1.E-05	2.E-03	6.E-05
6ij6	186	HIS	4.75%	1.E-05	2.E-06	2.E-01	8.E-01	3.E-03	2.E-04	1.E-03	4.E-08	5.E-02	7.E-07	1.E-05	2.E-05	4.E-05	5.E-04	2.E-07	7.E-04	3.E-05	1.E-04	3.E-04	9.E-06
5xjh	225	ASN	4.83%	2.E-03	2.E-04	5.E-02	3.E-06	6.E-01	2.E-04	5.E-06	1.E-06	9.E-06	8.E-06	4.E-04	3.E-06	3.E-04	7.E-08	1.E-06	4.E-02	3.E-01	2.E-08	2.E-08	2.E-04
5xjh	59	ARG	5.74%	7.E-03	6.E-02	2.E-01	6.E-02	3.E-03	1.E-01	2.E-01	2.E-04	2.E-02	3.E-03	3.E-03	9.E-02	6.E-03	3.E-03	1.E-04	5.E-02	2.E-01	2.E-04	3.E-03	3.E-02
5xjh	212	ASN	6.08%	3.E-01	1.E-02	6.E-02	3.E-01	2.E-03	6.E-03	2.E-02	7.E-04	4.E-04	2.E-04	3.E-03	3.E-02	9.E-04	1.E-04	3.E-05	3.E-01	7.E-03	2.E-05	1.E-04	9.E-04
6ij6	37	ASN	6.92%	4.E-05	5.E-05	7.E-02	9.E-01	1.E-04	1.E-05	2.E-04	5.E-07	9.E-05	5.E-06	3.E-06	2.E-04	5.E-06	2.E-06	8.E-07	5.E-04	6.E-05	2.E-07	2.E-06	2.E-05
6ij6	33	MET	7.37%	3.E-05	4.E-03	7.E-03	4.E-03	4.E-04	4.E-01	4.E-01	4.E-06	4.E-02	6.E-03	7.E-02	6.E-02	7.E-02	4.E-04	4.E-05	6.E-04	3.E-03	2.E-05	5.E-04	1.E-03

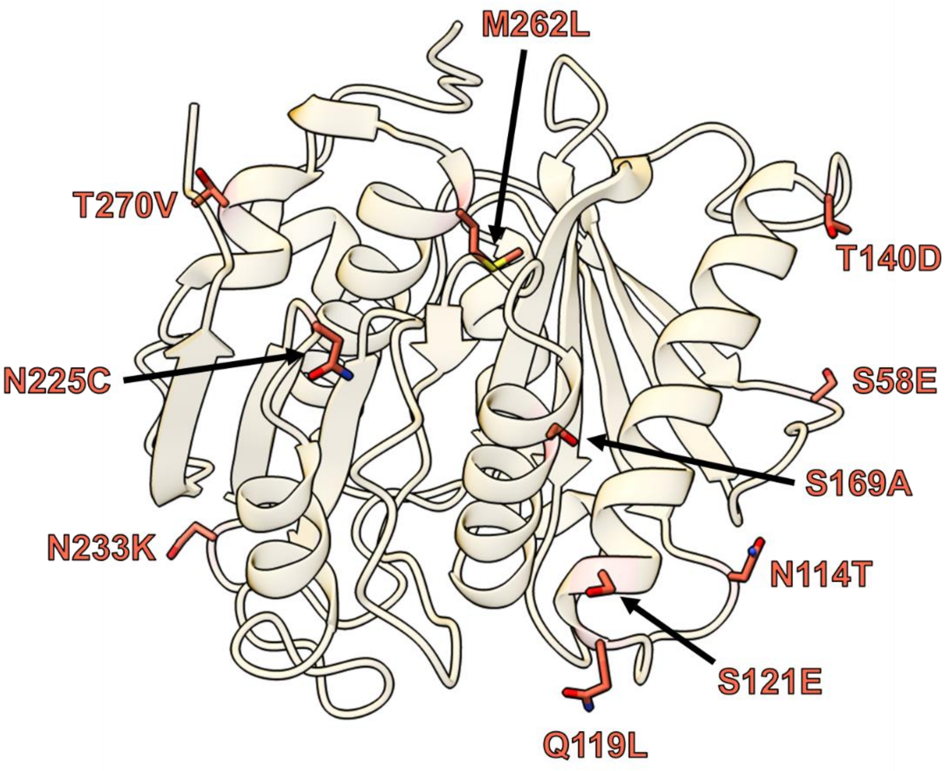
6ij6	279	THR	7.58%	7.E-03	1.E-02	4.E-02	2.E-01	2.E-03	2.E-02	3.E-01	6.E-05	1.E-02	1.E-02	3.E-03	8.E-02	3.E-03	2.E-03	9.E-05	1.E-01	8.E-02	2.E-04	1.E-03	3.E-02
5xjh	119	GLN	7.67%	1.E-05	5.E-03	1.E-03	3.E-04	1.E-04	8.E-02	7.E-03	2.E-04	7.E-03	3.E-05	1.E-01	1.E-01	5.E-01	1.E-01	1.E-06	2.E-05	5.E-05	3.E-03	3.E-02	8.E-06
5xjh	125	SER	8.20%	4.E-02	4.E-03	6.E-03	3.E-02	2.E-02	2.E-02	4.E-02	5.E-05	2.E-04	7.E-03	2.E-03	1.E-02	2.E-03	7.E-05	5.E-05	8.E-02	2.E-01	3.E-05	8.E-05	5.E-01
6ij6	212	ASN	8.26%	2.E-01	3.E-02	8.E-02	1.E-01	4.E-03	3.E-02	1.E-01	3.E-04	2.E-02	9.E-03	3.E-03	7.E-02	2.E-03	3.E-03	5.E-05	2.E-01	5.E-03	2.E-04	2.E-03	1.E-02
6ij6	87	TYR	8.43%	8.E-08	5.E-01	7.E-06	1.E-06	2.E-06	1.E-03	1.E-04	4.E-08	1.E-02	1.E-05	3.E-03	4.E-01	4.E-03	2.E-02	5.E-08	2.E-07	1.E-07	2.E-03	8.E-02	2.E-07
5xjh	82	ALA	8.52%	9.E-02	1.E-07	1.E-05	2.E-06	5.E-03	4.E-07	7.E-07	5.E-04	9.E-08	2.E-08	2.E-08	7.E-08	3.E-07	2.E-08	2.E-06	9.E-01	2.E-04	1.E-09	1.E-08	2.E-06
5xjh	117	LEU	8.68%	7.E-05	6.E-03	4.E-01	7.E-03	3.E-02	1.E-01	2.E-01	2.E-05	2.E-02	5.E-04	9.E-02	1.E-01	3.E-02	8.E-04	1.E-05	2.E-03	3.E-02	2.E-05	2.E-04	3.E-04
6ij6	104	HIS	9.20%	7.E-09	1.E-06	2.E-05	1.E-06	1.E-07	1.E-05	7.E-06	3.E-10	9.E-02	4.E-08	5.E-08	7.E-07	4.E-06	6.E-02	6.E-10	4.E-08	2.E-08	5.E-04	9.E-01	3.E-08
5xjh	213	SER	9.23%	2.E-02	2.E-02	3.E-02	1.E-01	1.E-03	3.E-02	2.E-01	9.E-05	5.E-04	5.E-03	2.E-02	7.E-02	3.E-03	2.E-04	5.E-05	9.E-02	3.E-01	8.E-05	4.E-04	3.E-02
6ij6	240	ALA	9.40%	9.E-02	2.E-05	1.E-03	9.E-05	8.E-01	3.E-04	1.E-04	1.E-05	1.E-05	3.E-04	7.E-05	4.E-05	2.E-04	1.E-06	3.E-05	7.E-03	6.E-02	8.E-07	9.E-07	2.E-02
6ij6	46	SER	9.48%	8.E-01	7.E-03	3.E-03	3.E-02	1.E-03	7.E-03	6.E-02	4.E-03	1.E-04	5.E-05	5.E-04	3.E-02	5.E-04	3.E-05	9.E-05	9.E-02	3.E-03	1.E-05	3.E-05	3.E-04
6ij6	270	THR	10.14%	2.E-05	2.E-03	2.E-03	6.E-04	3.E-04	5.E-03	4.E-03	3.E-07	7.E-05	2.E-01	1.E-03	1.E-02	8.E-04	4.E-06	2.E-06	1.E-04	1.E-01	1.E-06	3.E-06	6.E-01
6ij6	183	ALA	12.26%	1.E-01	3.E-04	2.E-01	1.E-02	3.E-01	2.E-02	3.E-02	8.E-05	1.E-04	8.E-05	2.E-05	9.E-05	2.E-02	5.E-06	1.E-04	2.E-01	1.E-01	4.E-06	8.E-06	1.E-02
6ij6	110	THR	12.30%	7.E-05	1.E-06	9.E-03	1.E-04	9.E-04	5.E-05	3.E-05	6.E-07	3.E-06	7.E-01	7.E-04	5.E-05	2.E-05	3.E-08	9.E-07	2.E-05	1.E-01	2.E-08	8.E-08	2.E-01
5xjh	270	THR	12.72%	5.E-03	1.E-04	3.E-03	6.E-04	7.E-03	4.E-03	3.E-04	3.E-05	3.E-05	3.E-02	1.E-03	5.E-04	6.E-04	8.E-06	6.E-03	5.E-03	1.E-01	8.E-07	6.E-06	8.E-01
6ij6	238	SER	13.39%	8.E-01	1.E-07	2.E-05	8.E-05	8.E-05	1.E-07	1.E-07	9.E-02	8.E-08	4.E-10	6.E-09	2.E-07	3.E-08	7.E-09	1.E-07	1.E-01	8.E-06	1.E-09	4.E-09	4.E-09
5xjh	124	SER	13.51%	9.E-01	2.E-09	2.E-07	1.E-07	6.E-05	4.E-08	2.E-08	7.E-06	5.E-08	7.E-12	3.E-10	2.E-09	2.E-08	1.E-09	3.E-09	1.E-01	9.E-07	3.E-11	8.E-10	5.E-10
6ij6	95	LYS	13.62%	5.E-07	9.E-04	1.E-03	1.E-04	3.E-05	2.E-01	6.E-01	2.E-09	9.E-04	3.E-05	6.E-02	1.E-01	3.E-03	7.E-06	1.E-08	5.E-06	9.E-06	3.E-07	3.E-06	4.E-06
5xjh	274	GLU	14.23%	2.E-06	1.E-03	3.E-03	3.E-04	9.E-04	5.E-02	1.E-01	8.E-08	1.E-02	3.E-03	7.E-02	3.E-02	6.E-01	8.E-02	6.E-07	8.E-06	7.E-04	4.E-05	6.E-03	8.E-03
6ij6	119	GLN	14.67%	8.E-07	2.E-02	7.E-05	3.E-05	1.E-05	1.E-01	2.E-03	5.E-06	5.E-03	2.E-05	1.E-02	1.E-01	2.E-01	3.E-01	2.E-07	9.E-07	2.E-06	1.E-02	2.E-01	1.E-06
5xjh	51	THR	15.48%	3.E-02	8.E-03	4.E-02	5.E-02	3.E-03	6.E-02	5.E-01	3.E-04	3.E-04	7.E-05	5.E-03	9.E-02	3.E-03	4.E-05	1.E-05	2.E-02	2.E-01	8.E-06	3.E-05	2.E-03
5xjh	41	ALA	16.64%	2.E-01	1.E-02	1.E-02	4.E-02	9.E-04	3.E-02	1.E-01	5.E-01	5.E-04	6.E-05	4.E-03	4.E-02	2.E-03	3.E-04	5.E-04	5.E-02	6.E-03	7.E-05	2.E-04	2.E-04
5xjh	92	SER	17.08%	8.E-01	2.E-03	9.E-04	1.E-02	2.E-04	2.E-03	2.E-02	4.E-05	7.E-06	1.E-05	3.E-05	2.E-03	3.E-05	2.E-06	5.E-05	2.E-01	1.E-03	1.E-06	4.E-06	1.E-04
5xjh	63	TYR	17.23%	4.E-09	7.E-06	5.E-07	7.E-09	2.E-07	2.E-06	8.E-08	1.E-09	5.E-03	3.E-09	3.E-07	9.E-07	7.E-05	8.E-01	2.E-10	1.E-08	1.E-08	2.E-04	2.E-01	8.E-09
5xjh	133	GLN	17.50%	4.E-06	3.E-05	4.E-02	2.E-02	1.E-04	2.E-01	7.E-01	1.E-07	8.E-04	2.E-03	6.E-03	1.E-03	1.E-03	2.E-05	8.E-07	1.E-05	1.E-02	2.E-06	1.E-05	8.E-03
6ij6	236	SER	18.79%	1.E-01	3.E-04	7.E-02	6.E-01	1.E-03	6.E-04	3.E-04	4.E-04	1.E-05	7.E-06	1.E-05	4.E-04	3.E-05	7.E-07	1.E-05	2.E-01	5.E-04	1.E-06	9.E-07	3.E-05
5xjh	292	GLU	19.20%	4.E-03	3.E-02	1.E-01	7.E-02	4.E-03	8.E-02	2.E-01	9.E-04	6.E-02	2.E-02	1.E-01	2.E-01	2.E-02	2.E-02	3.E-04	3.E-02	3.E-02	1.E-03	5.E-03	1.E-02

5xjh	208	ILE	19.53%	6.E-04	9.E-03	3.E-03	2.E-03	2.E-03	1.E-02	2.E-02	4.E-05	3.E-04	2.E-01	1.E-03	1.E-02	5.E-03	2.E-04	5.E-05	2.E-03	2.E-01	1.E-04	1.E-04	6.E-01
6ij6	269	SER	20.31%	5.E-01	3.E-04	6.E-02	1.E-01	8.E-03	1.E-02	7.E-03	3.E-05	2.E-03	1.E-03	2.E-04	2.E-03	2.E-04	2.E-05	7.E-06	2.E-01	4.E-02	4.E-06	3.E-05	8.E-03
6ij6	190	ASN	21.04%	5.E-07	8.E-06	2.E-01	8.E-01	3.E-05	4.E-05	1.E-04	3.E-08	4.E-07	3.E-07	5.E-07	2.E-05	1.E-06	2.E-08	2.E-08	4.E-05	1.E-05	1.E-08	1.E-08	2.E-06
6ij6	41	ALA	22.07%	2.E-01	4.E-02	3.E-02	6.E-02	6.E-04	9.E-02	4.E-01	1.E-04	9.E-03	6.E-04	6.E-03	1.E-01	2.E-03	1.E-03	6.E-05	3.E-02	3.E-02	5.E-04	1.E-03	2.E-03
5xjh	154	MET	22.55%	5.E-07	5.E-03	4.E-04	1.E-05	1.E-05	7.E-01	5.E-02	5.E-08	1.E-04	5.E-06	1.E-03	3.E-02	2.E-01	4.E-04	3.E-08	2.E-07	7.E-07	2.E-04	2.E-04	2.E-07
5xjh	207	SER	22.65%	8.E-02	1.E-02	2.E-01	4.E-01	8.E-03	8.E-03	4.E-02	5.E-04	5.E-03	2.E-04	5.E-04	6.E-03	2.E-03	6.E-04	7.E-05	2.E-01	1.E-02	8.E-05	7.E-04	1.E-03
5xjh	73	ASN	22.79%	5.E-06	4.E-06	2.E-01	8.E-01	2.E-04	2.E-04	2.E-03	2.E-07	3.E-05	3.E-06	3.E-06	4.E-05	3.E-06	2.E-07	4.E-07	4.E-04	2.E-05	3.E-08	2.E-07	1.E-05
6ij6	207	SER	23.23%	2.E-01	1.E-02	1.E-01	4.E-01	4.E-03	5.E-03	1.E-02	2.E-03	7.E-03	4.E-04	5.E-04	8.E-03	8.E-04	2.E-03	9.E-05	2.E-01	7.E-03	9.E-04	2.E-03	2.E-03
6ij6	261	PHE	23.26%	1.E-08	4.E-06	1.E-03	4.E-07	6.E-07	9.E-05	4.E-05	3.E-09	4.E-01	8.E-08	1.E-07	8.E-06	1.E-04	2.E-01	2.E-09	2.E-08	2.E-08	3.E-01	1.E-01	3.E-09
5xjh	190	ASN	23.32%	2.E-05	4.E-03	2.E-01	8.E-01	2.E-04	1.E-03	2.E-03	4.E-06	6.E-04	7.E-06	1.E-04	2.E-03	2.E-04	9.E-05	1.E-06	6.E-04	1.E-04	1.E-04	9.E-05	4.E-05
6ij6	165	GLY	25.56%	7.E-01	1.E-07	2.E-07	3.E-07	1.E-05	7.E-08	5.E-08	3.E-01	2.E-08	3.E-09	2.E-08	8.E-08	3.E-08	1.E-08	8.E-06	4.E-03	1.E-06	1.E-09	3.E-09	4.E-08
6ij6	125	SER	26.36%	9.E-02	3.E-03	1.E-03	4.E-03	6.E-03	1.E-02	2.E-02	1.E-04	3.E-04	2.E-03	2.E-03	1.E-02	1.E-03	2.E-04	6.E-05	3.E-01	4.E-01	5.E-05	2.E-04	2.E-01
6ij6	175	SER	26.87%	2.E-01	4.E-03	4.E-02	4.E-01	1.E-03	3.E-03	4.E-02	4.E-04	4.E-04	1.E-05	8.E-04	9.E-03	5.E-04	8.E-05	5.E-04	3.E-01	1.E-02	1.E-05	8.E-05	8.E-05
5xjh	37	ASN	27.55%	7.E-07	2.E-04	3.E-01	7.E-01	9.E-05	7.E-05	1.E-03	7.E-08	1.E-03	7.E-04	2.E-05	1.E-03	4.E-05	2.E-05	4.E-07	4.E-05	7.E-04	7.E-07	1.E-05	9.E-04
5xjh	287	ALA	27.60%	3.E-01	4.E-03	9.E-03	2.E-01	7.E-03	4.E-03	2.E-02	2.E-03	4.E-03	2.E-05	2.E-04	2.E-02	1.E-03	3.E-04	3.E-05	5.E-01	6.E-03	1.E-04	3.E-04	8.E-04
6ij6	63	TYR	27.81%	8.E-09	5.E-06	3.E-06	2.E-08	6.E-07	1.E-05	2.E-07	3.E-09	2.E-02	8.E-09	1.E-06	1.E-06	2.E-04	7.E-01	6.E-10	3.E-08	5.E-08	3.E-04	3.E-01	2.E-08
6ij6	231	GLU	28.31%	3.E-06	3.E-04	3.E-03	3.E-05	5.E-03	7.E-01	3.E-01	4.E-08	2.E-06	2.E-06	1.E-03	5.E-03	8.E-03	1.E-08	1.E-08	9.E-05	1.E-06	6.E-08	9.E-09	5.E-07
6ij6	133	GLN	28.50%	3.E-06	2.E-04	4.E-02	1.E-01	9.E-05	3.E-01	5.E-01	3.E-07	5.E-03	6.E-04	5.E-03	4.E-03	2.E-03	7.E-05	1.E-06	1.E-05	1.E-03	8.E-06	7.E-05	6.E-03
5xjh	159	TRP	28.75%	1.E-10	3.E-05	3.E-07	1.E-07	9.E-09	8.E-06	4.E-07	5.E-11	3.E-02	3.E-10	9.E-07	3.E-05	3.E-05	3.E-01	5.E-11	6.E-10	3.E-10	3.E-01	3.E-01	4.E-10
6ij6	132	ARG	29.00%	3.E-05	3.E-01	4.E-03	1.E-03	8.E-05	4.E-01	3.E-02	7.E-07	6.E-02	7.E-05	5.E-04	8.E-02	1.E-02	3.E-02	1.E-06	4.E-05	4.E-04	6.E-02	2.E-02	2.E-04
5xjh	175	SER	29.89%	5.E-01	8.E-03	1.E-02	1.E-01	2.E-03	1.E-02	4.E-02	1.E-04	3.E-04	2.E-05	2.E-03	3.E-02	8.E-04	8.E-05	1.E-05	3.E-01	1.E-02	1.E-05	7.E-05	3.E-04

Supplementary Information Fig. 2 | Disfavored PETase residues flagged by MutCompute from the wild-type and ThermoPETase crystal structures. MutCompute outputs a probability distribution that describes the likelihood of each of the 20 canonical amino acids to be the wild-type amino acid for the surrounding chemical environment. A disfavored residue is defined as a residue where the amino acid with the highest predicted probability is not the wild-type amino acid. Here, a 30% wild-type probability cutoff was used to down select disfavored residues**.**

Ranking	position	wtAA	prAA	wt_prob	pred_prob	avg_log_ratio
1	121	SER	GLU	0.11%	61.20%	6.86
2	262	MET	LEU	4.12%	66.51%	4.77
3	233	ASN	LYS	4.86%	55.93%	3.06
4	140	THR	ASP	14.23%	75.20%	2.69
5	58	SER	GLU	5.22%	45.81%	2.49
6	169	SER	ALA	10.29%	89.60%	2.46
7	119	GLN	LEU	6.06%	54.65%	2.40
8	225	ASN	CYS	7.94%	78.08%	2.31
9	270	THR	VAL	8.65%	72.13%	2.26
10	114	ASN	THR	9.53%	76.00%	2.14
11	91	GLN	ILE	10.03%	53.89%	2.14
12	207	SER	ASP	15.83%	37.06%	1.78
13	212	ASN	ALA	6.17%	33.75%	1.73
14	59	ARG	ASN	6.26%	34.64%	1.69
15	136	SER	LEU	5.99%	28.02%	1.66
16	279	THR	GLU	6.85%	26.04%	1.66
17	168	ILE	LEU	28.37%	71.44%	1.65
18	263	ASP	ASN	19.55%	32.91%	1.65
19	154	MET	GLN	10.19%	46.02%	1.64
20	190	ASN	ASP	21.64%	77.84%	1.62
21	201	PHE	LEU	24.70%	67.93%	1.61
22	124	SER	ALA	25.46%	74.53%	1.32
23	208	ILE	VAL	18.96%	49.48%	1.23
24	117	LEU	LYS	9.84%	25.37%	1.21
25	95	LYS	GLU	20.94%	44.44%	1.11
26	73	ASN	ASP	28.55%	70.65%	1.06
27	53	ARG	LYS	29.40%	66.87%	1.00
28	274	GLU	MET	22.29%	46.47%	0.99
29	67	THR	VAL	29.74%	50.17%	0.97
30	125	SER	ALA	18.70%	38.47%	0.59
31	213	SER	THR	27.53%	40.39%	0.35
32	146	TYR	HIS	27.67%	44.27%	0.34
33	88	THR	THR	22.54%	22.54%	0.00
34	172	ASN	ASN	25.92%	25.92%	0.00
35	187	SER	SER	27.74%	27.74%	0.00
36	292	GLU	GLU	29.43%	29.43%	0.00
37	152	ALA	GLY	22.79%	35.05%	-0.10

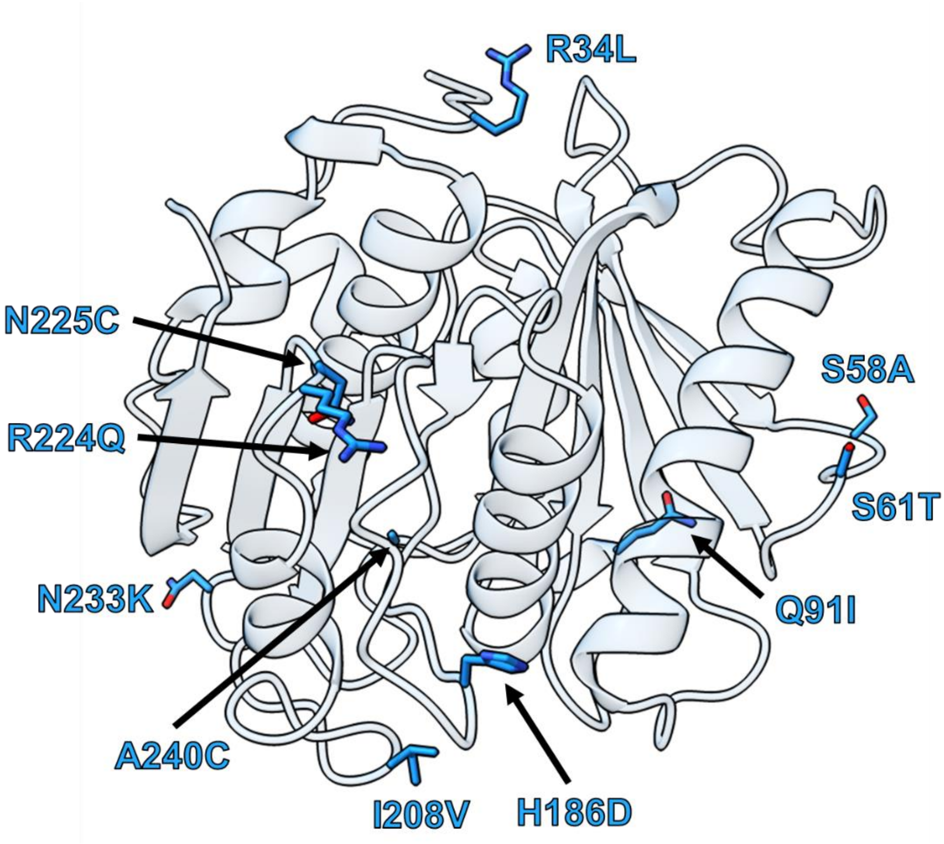
Supplementary Information Fig. 3a | Predictions (based on wild-type PETase) ranked by fold change in the probabilities between the predicted and the wild-type amino acid. Fold change predictions are provided as a means of down-selecting potential mutations.



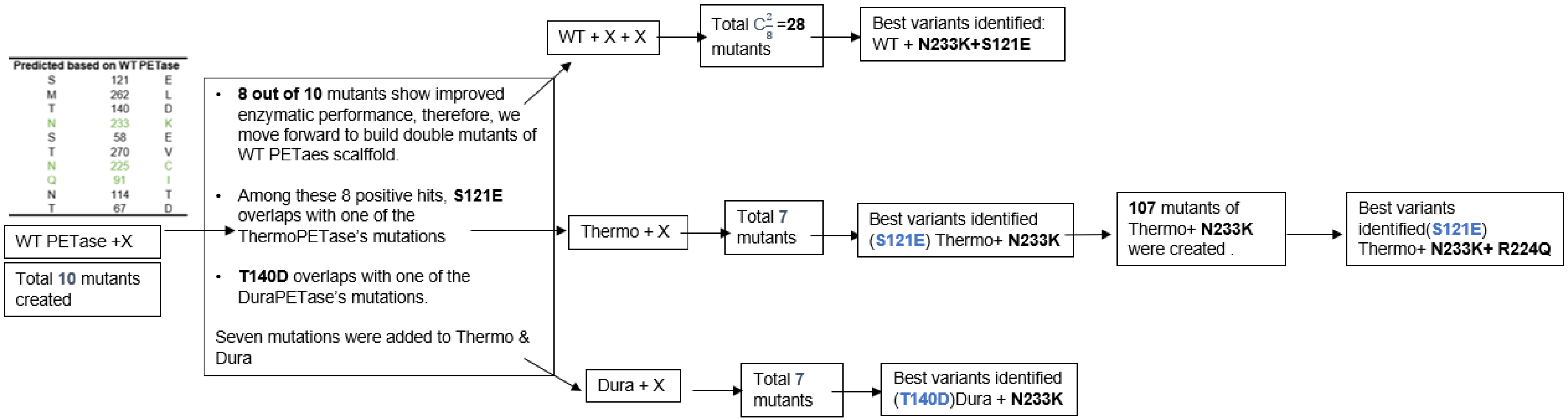
Supplementary Information Fig. 3b | TOP 10 ranked predictions (based on wild-type PETase). The top 10 mutations predicted for the wild-type PETase scaffold are presented.

Ranking	position	wtAA	prAA	wt_prob	pred_prob	avg_log_ratio
1	91	GLN	ILE	0.09%	98.29%	7.42
2	233	ASN	LYS	0.09%	97.29%	7.39
3	225	ASN	CYS	0.32%	98.01%	5.86
4	61	SER	THR	0.54%	31.85%	3.78
5	208	ILE	VAL	3.02%	88.68%	3.57
6	58	SER	ALA	2.30%	78.28%	3.54
7	34	ARG	LEU	2.99%	78.89%	3.41
8	240	ALA	CYS	9.40%	81.59%	3.24
9	186	HIS	ASP	4.75%	77.21%	3.20
10	224	ARG	GLN	3.52%	39.61%	3.14
11	53	ARG	LYS	2.82%	56.07%	2.99
12	270	THR	VAL	10.14%	63.14%	2.91
13	136	SER	THR	4.15%	66.37%	2.82
14	37	ASN	ASP	6.92%	92.96%	2.65
15	104	HIS	TYR	9.20%	85.21%	2.33
16	46	SER	ALA	9.48%	75.76%	2.31
17	95	LYS	GLU	13.62%	57.80%	2.22
18	59	ARG	THR	3.25%	31.60%	2.18
19	87	TYR	ARG	8.43%	50.29%	2.14
20	238	SER	ALA	13.39%	78.03%	2.09
21	236	SER	ASP	18.79%	61.12%	1.82
22	110	THR	ILE	12.30%	69.39%	1.75
23	33	MET	GLN	7.37%	36.75%	1.69
24	165	GLY	ALA	25.56%	74.08%	1.55
25	279	THR	GLU	7.58%	31.98%	1.44
26	119	GLN	PHE	14.67%	29.22%	1.35
27	190	ASN	ASP	21.04%	78.93%	1.33
28	63	TYR	PHE	27.81%	69.99%	1.32
29	212	ASN	ALA	8.26%	23.24%	1.10
30	269	SER	ALA	20.31%	54.77%	0.98
31	231	GLU	GLN	28.31%	69.43%	0.93
32	133	GLN	GLU	28.50%	52.67%	0.80
33	183	ALA	CYS	12.26%	30.00%	0.74
34	175	SER	ASP	26.87%	42.64%	0.71
35	41	ALA	GLU	22.07%	38.13%	0.55
36	261	PHE	HIS	23.26%	37.42%	0.52
37	125	SER	THR	26.36%	39.71%	0.47
38	207	SER	ASP	23.23%	44.12%	0.46
39	132	ARG	GLN	29.00%	41.70%	0.37
40	277	ASN	ASN	23.99%	23.99%	0.00

Supplementary Information Fig. 3c | Predictions (based on ThermoPETase) ranked by fold change in the probabilities between the predicted and the wild-type amino acid. Fold change predictions are provided as a means of down-selecting potential mutations.



Supplementary Information Fig. 3d | TOP 10 ranked predictions (based on ThermoPETase). The top 10 mutations predicted for the ThermoPETase scaffold are presented.

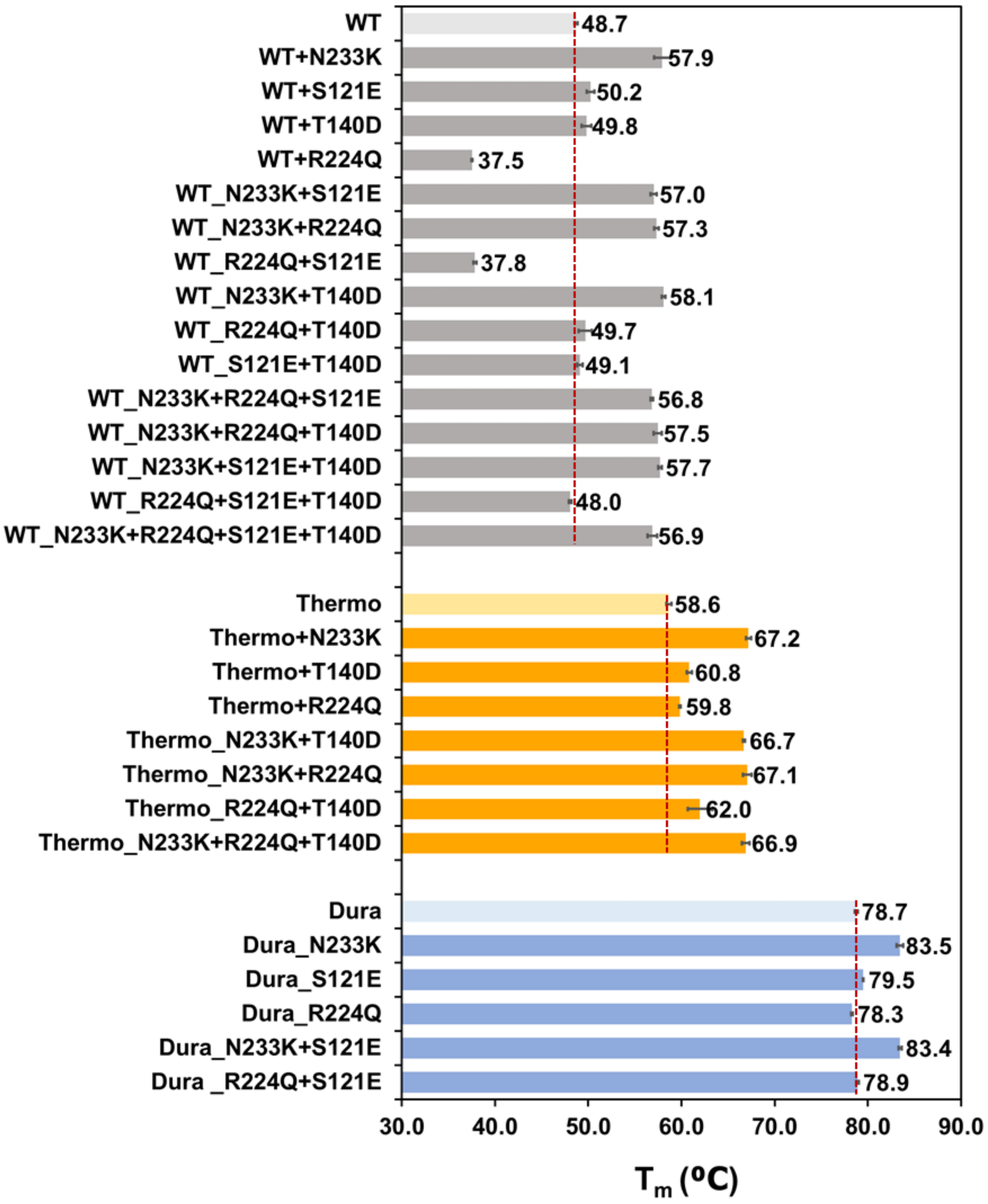


Supplementary Information Fig. 4 | Selecting mutations based on experimental catalytic activity measurements. A scheme for selecting mutations based on experimental evidence is provided.

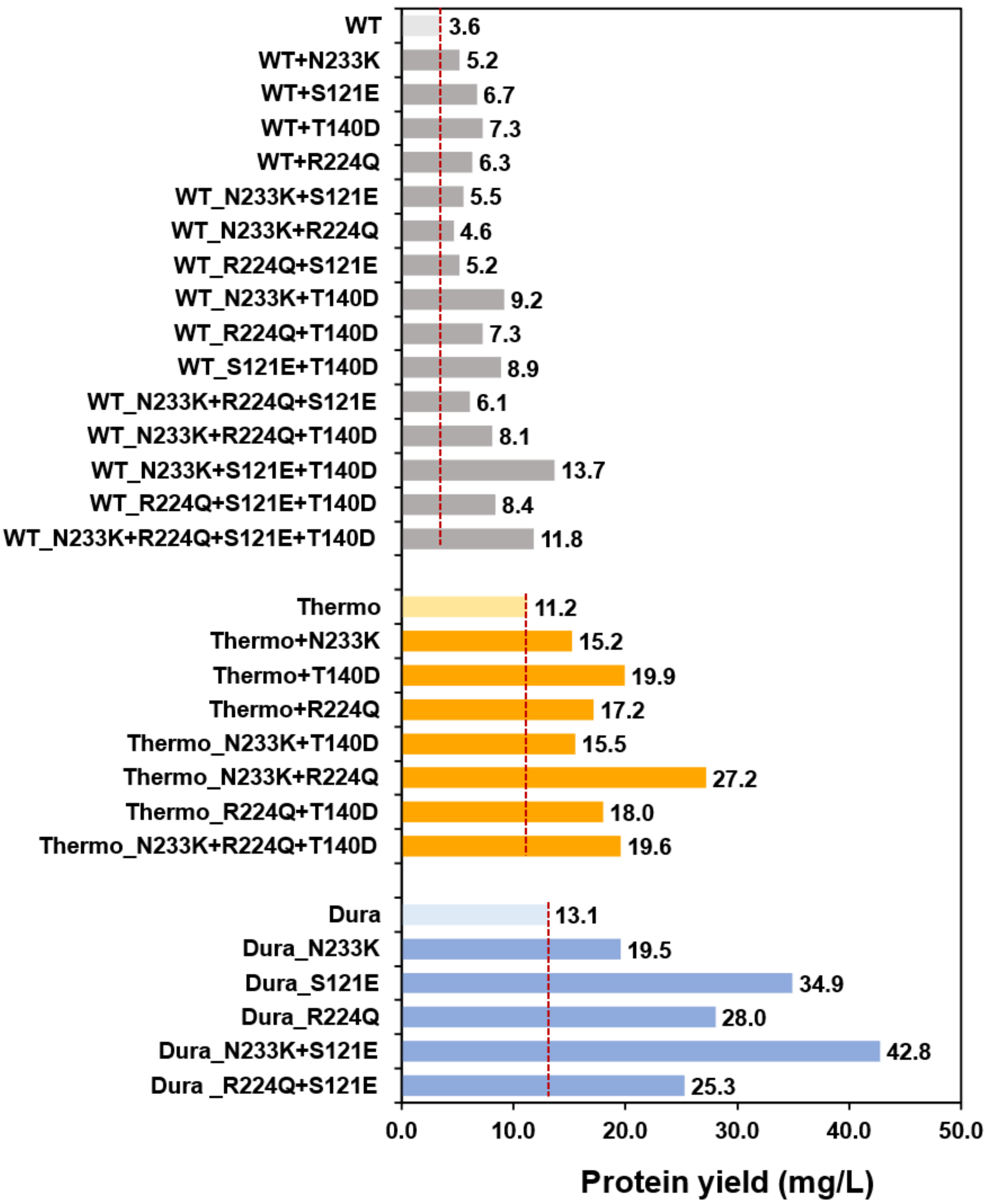
Initially, we chose the top ten ranked predictions based on crystal structure PDB: 5XJH (Supplementary Information Fig. 3a) and introduced them respectively into the wild-type PETase scaffold to generate ten single mutants. Experimental characterization of these variants showed that eight out of these ten predicted mutations confer improved thermostability and activity to the wild-type PETase scaffold. Notably, of such eight beneficial mutations, S121E and T140D are each overlapped with one of the mutations of ThermoPETase and DuraPETase.

Subsequently, we paired two of the eight beneficial mutations to create all 28 possible double mutants of wild-type PETase. Meanwhile, the unique beneficial mutations were respectively introduced into ThermoPETase and DuraPETase scaffolds to generate 14 variants that contain two predictions from Mutcompute. Among these 42 variants, the best variants identified for each scaffold all contain the predicted mutation-N233K. As the variant exhibiting the highest enzymatic activity, ThermoPETase^{N233K} was chosen as the template for further mutagenesis.

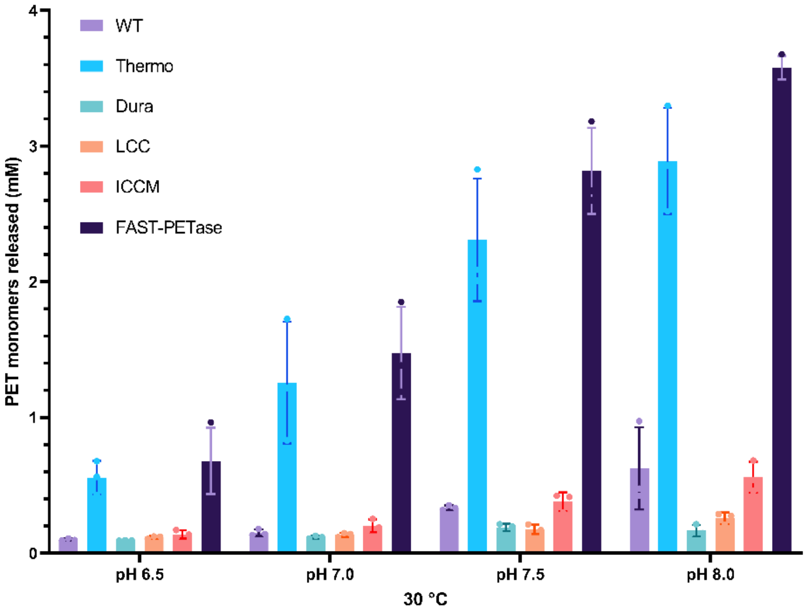
Finally, a total of 107 variants of ThermoPETase^{N233K} were created by incorporating single or multiple mutations from the 14 top ranked predictions based on both crystal structures PDB: 5XJH and 6IJ6 as well as lower ranked predictions selected by a rational design strategy. After comparative analysis of the enzymatic performance of these 107 variants, ThermoPETase$^{N233K/R224Q}$ was identified as the best variant as it showed improved activity versus ThermoPETase^{N233K}. Given the synergetic interactions among the four predicted mutations that resulted in the best WT PETase, ThermoPETase and DuraPETase variants, S121E, N233K, R224Q and T140D were further selected for combinatorial assembly and follow-up analysis.



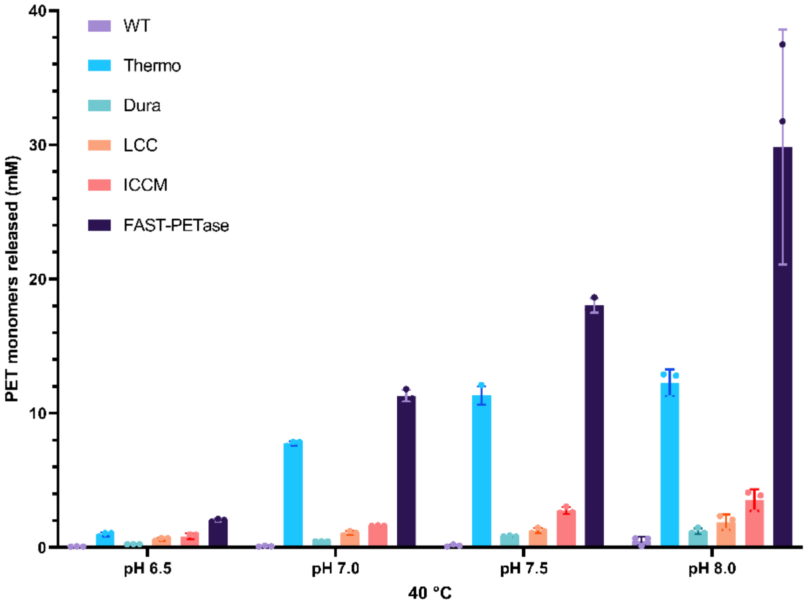
Supplementary Information Fig. 5 | Thermostability of the PETase variants incorporating the mutations predicted by Mutcompute and their respective scaffolds—wild-type PETase (WT), ThermoPETase (Thermo), DuraPETase (Dura). The melting temperature of each enzyme was determined by DSC. All measurement were conducted in triplicate (n=3).



Supplementary Information Fig. 6 | Protein yield of the PETase variants incorporating the mutations predicted by Mutcompute and their respective scaffolds—wild-type PETase (WT), ThermoPETase (Thermo), DuraPETase (Dura). Protein yields from *P. putida* purification experiments indicate improved yields from mutant enzymes.

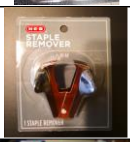


a



b

Supplementary Information Fig. 7 | The PET-hydrolytic activity of FAST-PETase outperformed various PHEs at mild temperatures and modest pH. Comparison of PET-hydrolytic activity of FAST-PETase, wild-type PETase (WT), ThermoPETase (Thermo), DuraPETase (Dura), LCC and ICCM across a range of pH (6.5 – 8.0) at reaction temperatures of 30 ºC (**a.**) and 40 ºC (**b.**). PET-hydrolytic activity was evaluated by measuring the amount of PET monomers (the sum of TPA and MHET) released from hydrolyzing gf-PET film by the tested enzymes after 96 hrs of reaction time. All measurement were conducted in triplicate (n=3).

Sample number	Postconsumer Plastic products	Initial mass (mg)	Crystallinity %	Time for complete degradation (days)	Category	Mn kg/mol	Mw kg/mol	Đ
#1		9.49 ± 0.27	1.18% ± 0.02%	2.5	Medication packaging	30.2	55.4	1.83
#2		6.36 ± 0.07	1.21% ± 0.09%	2.5	Household goods packaging	31.6	56.2	1.78
#3		16.27 ± 0.52	1.23% ± 0.20%	4.5	Beverage packaging	30.7	53.9	1.76
#4		12.34 ± 0.11	1.30% ± 0.14%	4	Household goods packaging	33.1	61.2	1.85
#5		8.28 ± 0.48	1.40% ± 0.14%	2	Food packaging	29.2	50.9	1.74
#6		15.75 ± 0.11	1.42% ± 0.29%	4.5	Food packaging	29.0	50.9	1.76
#7		4.86 ± 0.32	1.44% ± 0.25%	2	Household goods packaging	29.8	57.9	1.94
#8		10.57 ± 0.02	1.50% ± 0.21%	3.5	Food packaging	33.2	59.9	1.80
#9		6.41 ± 0.23	1.54% ± 0.13%	2.5	Office supplies packaging	32.1	56.8	1.77
#10		8.76 ± 0.24	1.55% ± 0.22%	2	Office supplies packaging	35.4	66.6	1.88

Supplementary Information Fig. 8 | Mass, crystallinity %, molecular weights (Mn, Mw), polydispersity indices (Đ) and time for complete degradation of various pc-PET films by FAST-PETase. The circular pc-PET films (6 mm in diameter) were hole-punched from 51 different post-consumer plastic products used in the packaging of food, beverages, medications, office supplies, household goods and cosmetics available at local grocery store chains (Walmart, Costco, and HEB). The pc-PET films were hydrolysed by serial treatment with FAST-PETase at 50 ºC until the films were completed degraded. The enzyme solution (200 nM of FAST-PETase in 100mM KH_2PO4-NaOH (pH 8.0) buffer) was replenished every 24 hours. The crystallinity % of the intact pc-PET films was determined by DSC. The initial mass of the films was determined gravimetrically by a digital scale. Both DSC and gravimetric measurements were conducted in triplicate. Means ± s.d. (n=3) are shown.

Sample number	Postconsumer Plastic products	Initial mass (mg)	Crystallinity %	Time for complete degradation (days)	Category	Mn kg/mol	Mw kg/mol	Đ
#11		9.46 ± 0.2	1.65% ± 0.08%	2.5	Food packaging	33.3	60.6	1.82
#12		10.20 ± 0.5	1.65% ± 0.21%	2.5	Cosmetics packaging	27.2	50.3	1.85
#13		11.54 ± 0.27	1.68% ± 0.30%	4	Food packaging	32.6	59.8	1.83
#14		15.44 ± 0.25	1.68% ± 0.06%	5	Food packaging	27.1	48.2	1.78
#15		13.06 ± 0.72	1.73% ± 0.27%	2.5	Medication packaging	28.2	52.3	1.85
#16		11.84 ± 1.06	2.00% ± 0.16%	5	Medication packaging	23.3	45.3	1.94
#17		4.37 ± 0.66	2.01% ± 0.03%	1	Food packaging	30.9	54.7	1.77
#18		17.13 ± 0.17	2.14% ± 0.21%	4.5	Office supplies packaging	36.4	62.4	1.71
#19		10.83 ± 0.69	2.19% ± 0.22%	1.5	Household goods packaging	36.1	62.5	1.73
#20		11.25 ± 0.25	2.19% ± 0.07%	3.5	Food packaging	26.0	52.4	2.02
#21		14.34 ± 0.1	2.20% ± 0.17%	3.5	Household goods packaging	24.0	44.1	1.84

Supplementary Information Fig. 8 continued

Sample number	Postconsumer Plastic products	Initial mass (mg)	Crystallinity %	Time for complete degradation (days)	Category	Mn kg/mol	Mw kg/mol	Đ
#22		17.06 ± 0.74	2.28% ± 0.24%	7	Cosmetics packaging	36.2	66.3	1.83
#23		11.27 ± 0.71	2.29% ± 0.13%	4	Food packaging	24.8	61.5	2.48
#24		7.07 ± 0.12	2.45% ± 0.17%	2.5	Food packaging	28.1	50.9	1.81
#25		11.06 ± 0.08	2.49% ± 0.26%	5	Medication packaging	33.4	61.1	1.83
#26		9.34 ± 0.28	2.53% ± 0.22%	4	Medication packaging	32.7	57.8	1.77
#27		10.52 ± 0.07	2.53% ± 1.64%	5	Household goods packaging	32.7	59.9	1.83
#28		8.97 ± 0.37	2.56% ± 0.16%	4	Food packaging	28.7	53.7	1.87
#29		13.04 ± 0.03	2.56% ± 0.24%	6	Office supplies packaging	33.7	62.3	1.85
#30		8.16 ± 2.23	2.61% ± 1.05%	3.5	Food packaging	38.0	70.8	1.86
#31		13.23 ± 0.49	2.67% ± 0.30%	2	Household goods packaging	31.3	55.1	1.76
#32		20.92 ± 0.2	2.71% ± 0.14%	7	Food packaging	32.5	58.3	1.79

Supplementary Information Fig. 8 continued

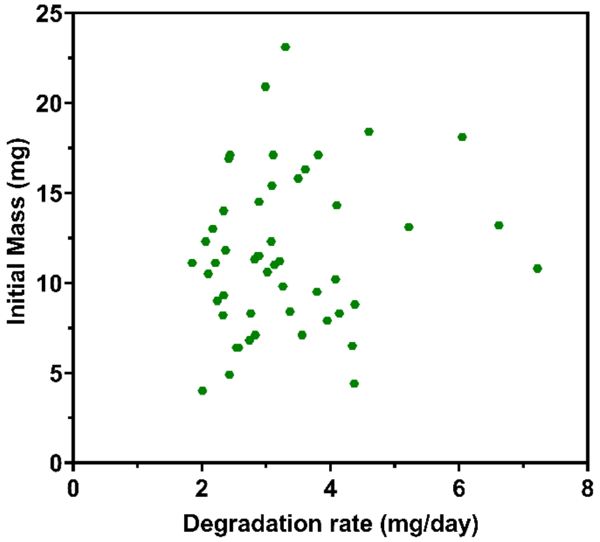
Sample number	**Postconsumer Plastic products**	**Initial mass (mg)**	**Crystallinity %**	**Time for complete degradation (days)**	**Category**	**Mn kg/mol**	**Mw kg/mol**	**Đ**
#33		18.4 ± 0.1	2.90% ± 0.16%	4	Household goods packaging	28.7	52.4	1.83
#34		7.12 ± 1.16	2.93% ± 0.02%	2	Household goods packaging	36.8	67.7	1.84
#35		8.27 ± 1.84	3.00% ± 0.61%	3	Food packaging	28.3	50.2	1.77
#36		18.14 ± 0.13	3.06% ± 0.30%	3	Household goods packaging	29.8	52.7	1.77
#37		9.79 ± 0.06	3.21% ± 0.27%	3	Beverage packaging	33.2	57.5	1.73
#38		4.01 ± 0.54	3.42% ± 0.45%	2	Food packaging	30.9	56.1	1.82
#39		6.84 ± 0.45	3.47% ± 0.67%	2.5	Beverage packaging	35.7	64.1	1.80
#40		11.08 ± 0.77	3.56% ± 0.66%	6	Food packaging	39.7	68.7	1.73
#41		14.04 ± 0.4	3.57% ± 0.16%	6	Food packaging	31.8	57.0	1.79
#42		8.43 ± 0.48	3.58% ± 0.19%	2.5	Household goods packaging	31.2	58.0	1.86
#43		12.34 ± 0.3	3.72% ± 0.24%	6	Office supplies packaging	36.0	66.5	1.85

Supplementary Information Fig. 8 continued

Sample number	Postconsumer Plastic products	Initial mass (mg)	Crystallinity %	Time for complete degradation (days)	Category	Mn kg/mol	Mw kg/mol	Đ
#44		14.46 ± 0.43	4.09% ± 0.18%	5	Food packaging	31.4	56.2	1.79
#45		16.94 ± 0.12	4.56% ± 0.26%	7	Food packaging	34.5	62.7	1.82
#46		7.9 ± 2.78	4.69% ± 1.08%	2	Food packaging	31.6	55.7	1.76
#47		11.49 ± 0.2	4.85% ± 0.36%	4	Household goods packaging	35.1	64.1	1.83
#48		17.12 ± 0.16	4.85% ± 1.08%	5.5	Food packaging	33.1	57.9	1.75
#49		6.51 ± 2.65	5.30% ± 0.18%	1.5	Cosmetics packaging	28.8	50.9	1.77
#50		10.96 ± 0.21	5.79% ± 0.11%	3.5	Household goods packaging	32.6	58.8	1.80
#51		23.1 ± 0.05	6.24% ± 0.25%	7	Toy packaging	32.2	59.8	1.86

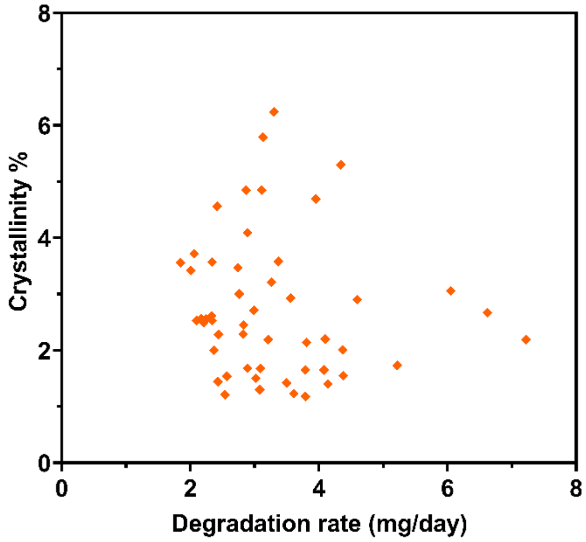
Supplementary Information Fig. 8 continued

a



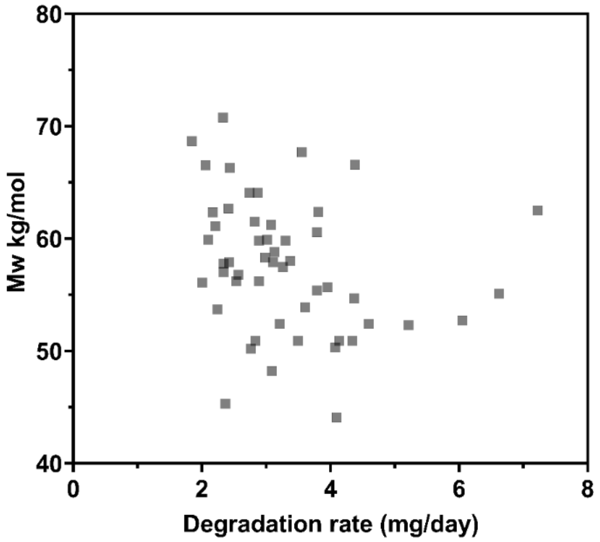
Initial Mass (mg)
25
20
15
10
5
0
0
2
4
6
8
Degradation rate (mg/day)

b



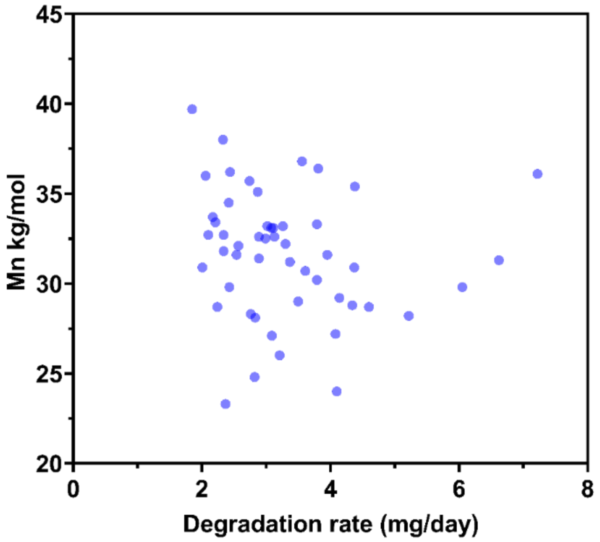
Crystallinity %
8
6
4
2
0
0
2
4
6
8
Degradation rate (mg/day)

c

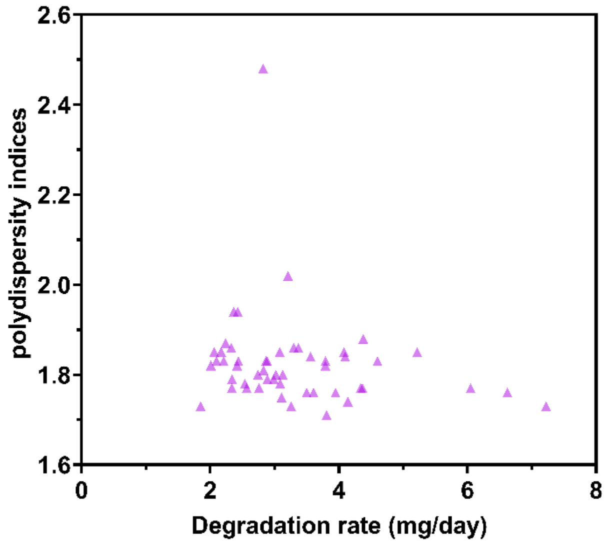


Mw kg/mol
80
70
60
50
40
0
2
4
6
8
Degradation rate (mg/day)

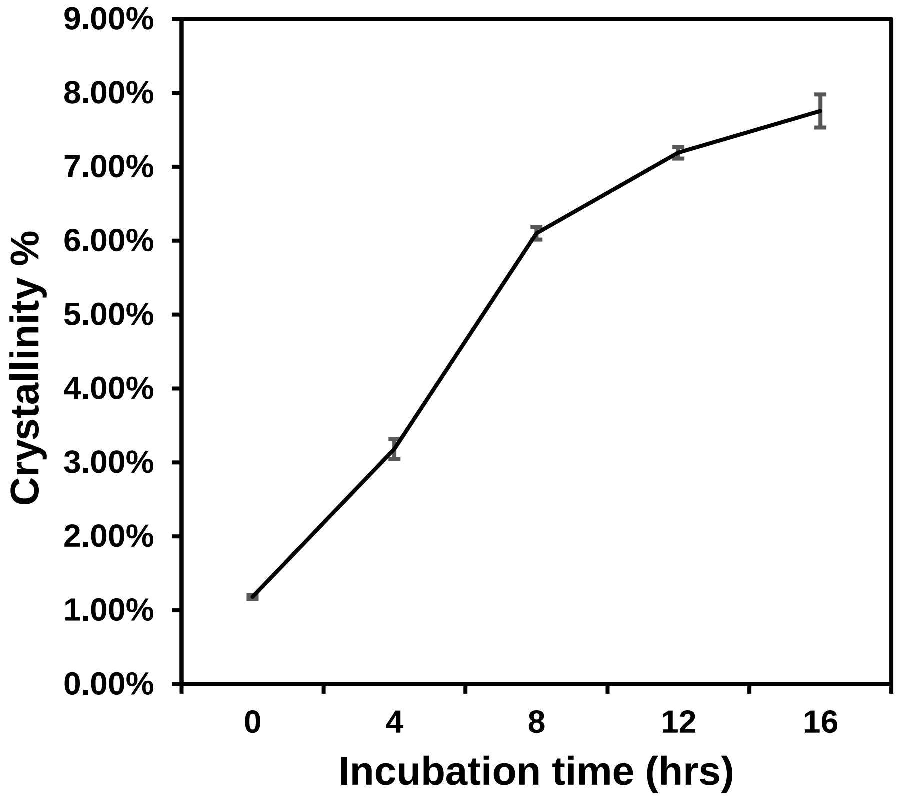
d



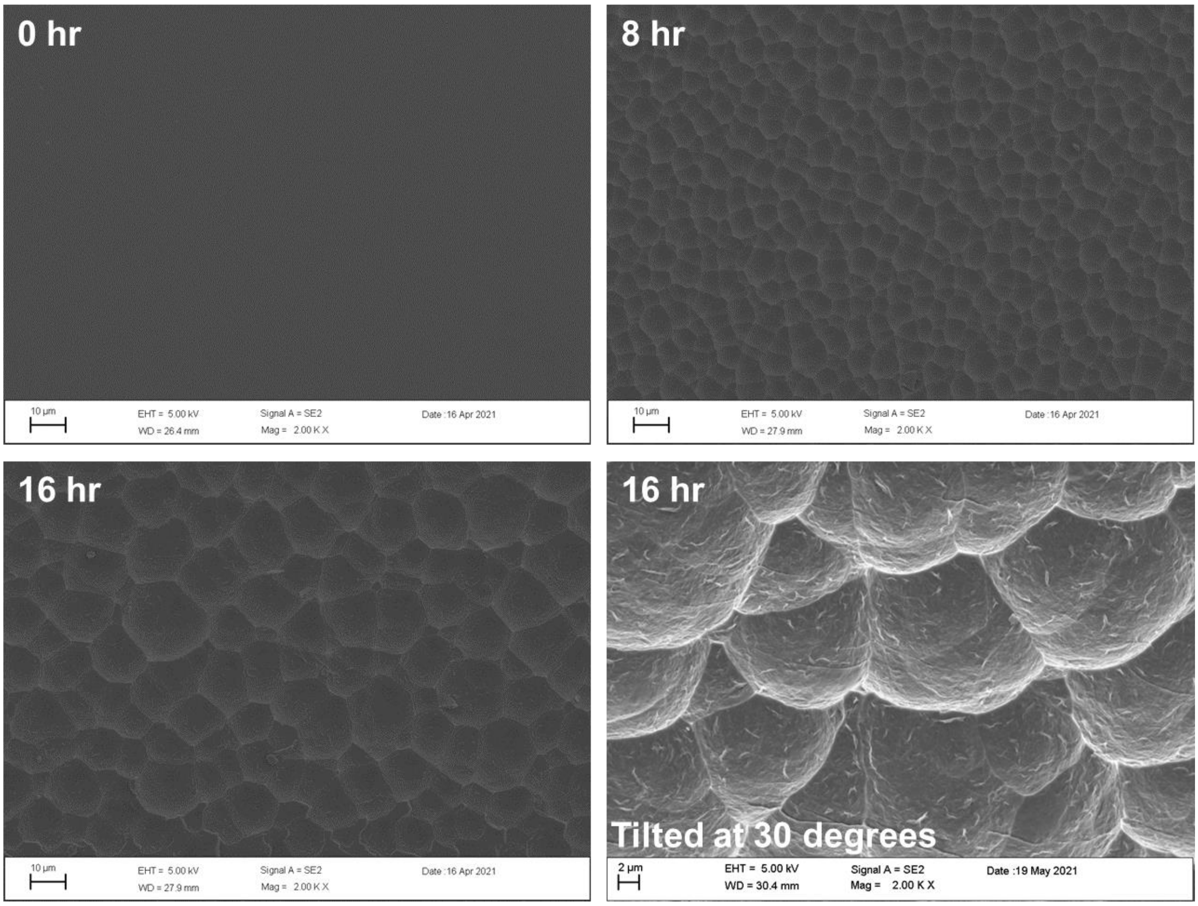
e



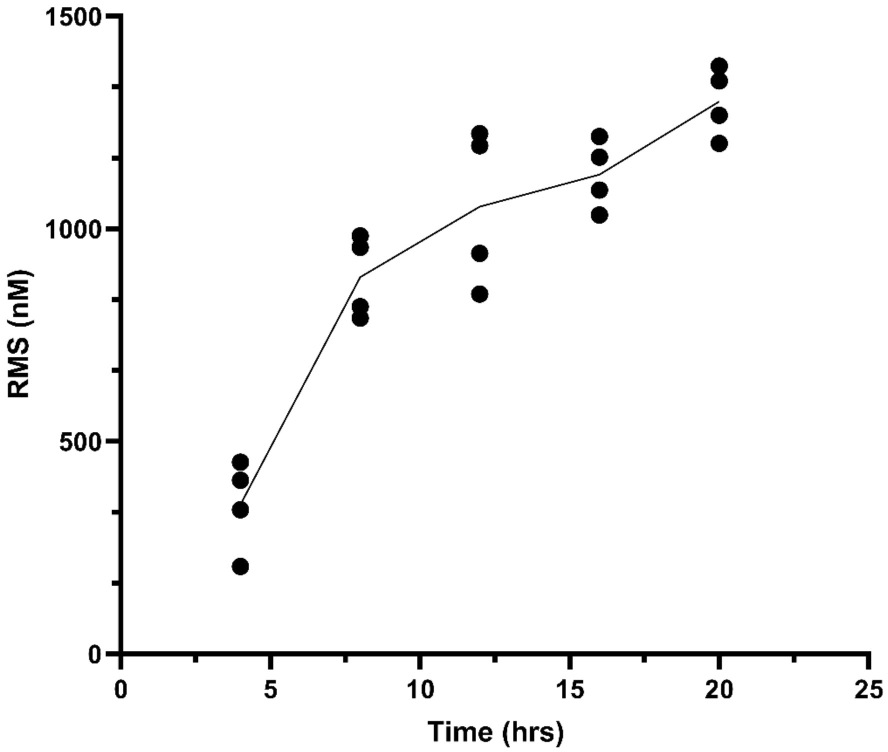
Supplementary Information Fig. 9 | Scatterplot of degradation rate versus (a.) initial mass or (b.) crystallinity % or (c.) weight average molecular weight (Mw) or (d.) number average molecular weight (Mn) or (e.) polydispersity indices of the hole-punched films from 51 different post-consumer plastic products. Degradation rate was not found to be dependent on any one metric of these various plastics.



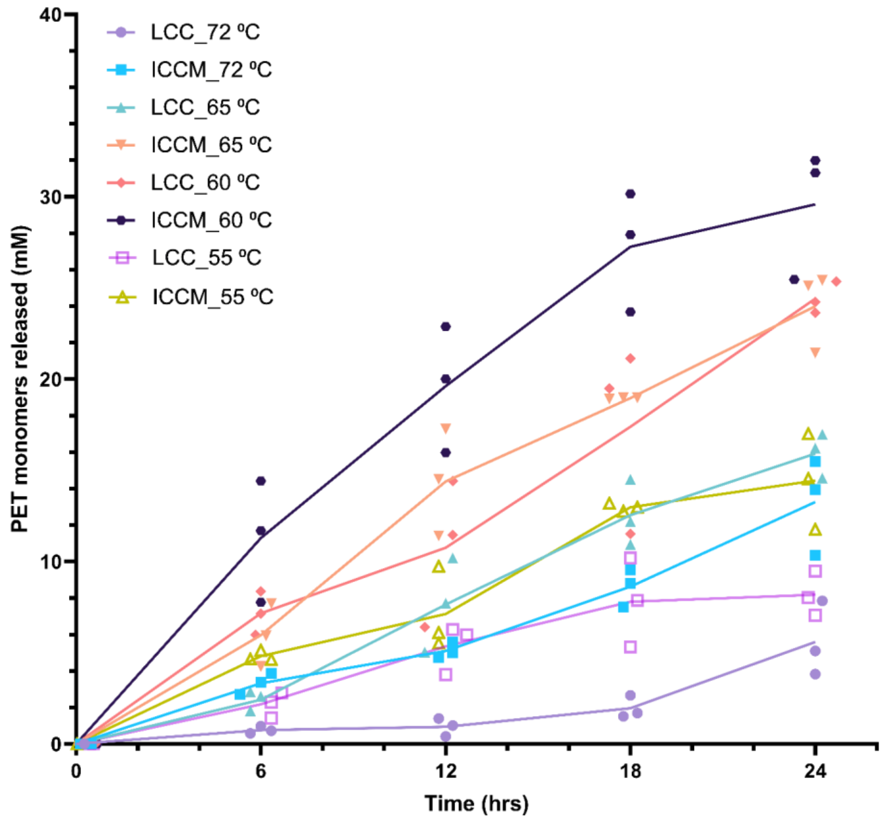
Supplementary Information Fig. 10 | Time-course of crystallinity % of the degraded pc-PET film. The hole-punched PET films from a bean cake PET container were treated with FAST-PETase for 0 hr, 4hr, 8 hr,12 hrs 16 hr in 100 mM KH_2PO_4-NaOH (pH 8.0) buffer at 50 ºC. Crystallinity % of the films was determined by DSC. All measurement were conducted in duplicate (n=2).



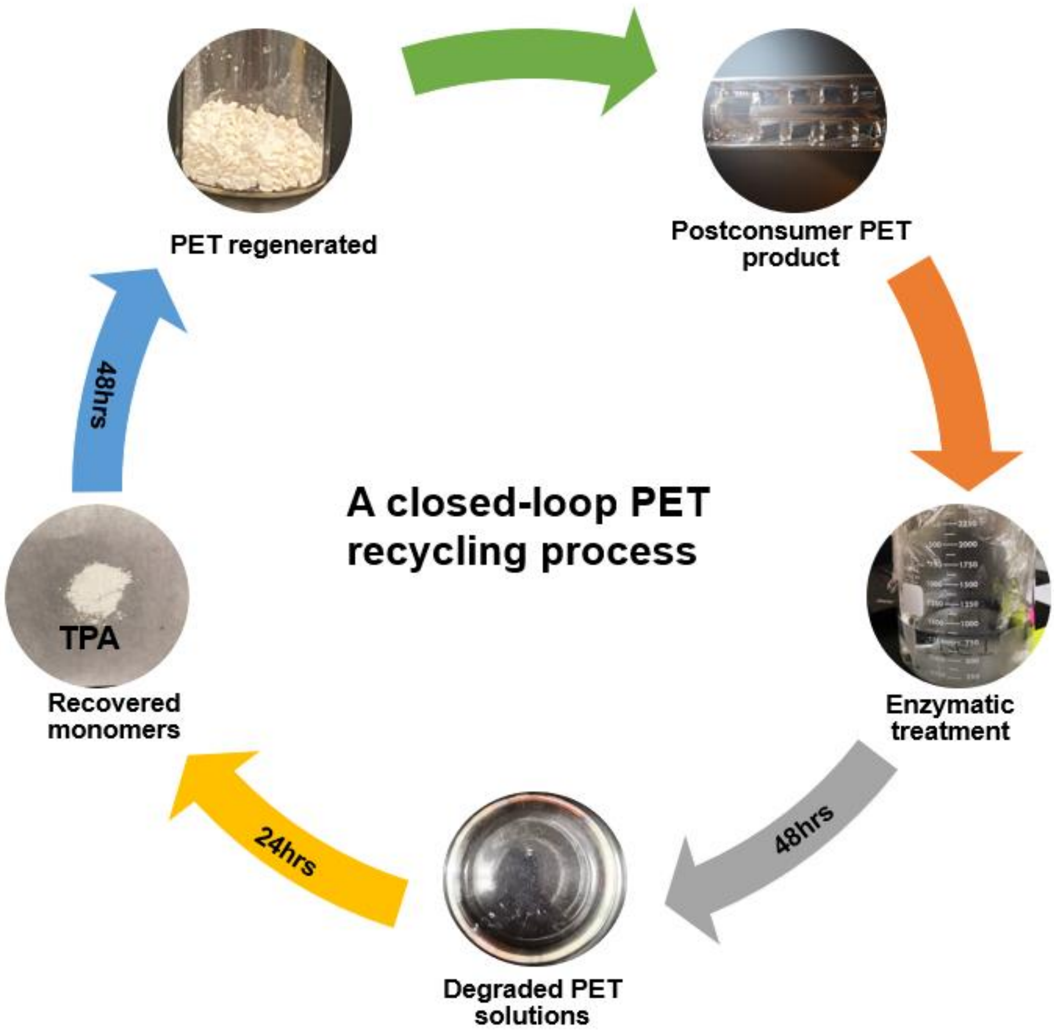
Supplementary Information Fig. 11 | Scanning electron microscopic analysis of the pc-PET films. The hole-punched PET films from a bean cake PET container were treated with FAST-PETase for 0 hr, 8 hr, 16 hr in 100 mM KH_2PO_4-NaOH (pH 8.0) buffer at 50 ºC.



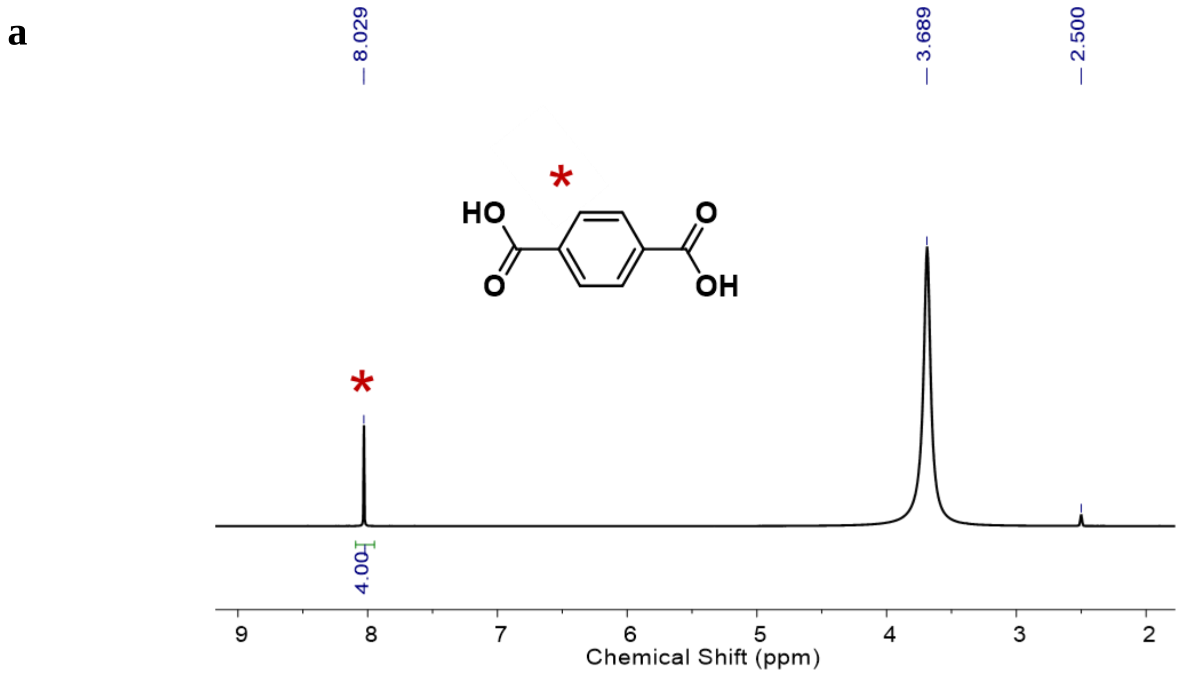
Supplementary Information Fig. 12 | The surface roughness of the pc-PET films determined by atomic force microscopy. The hole-punched PET films from a bean cake PET container were treated with FAST-PETase for 4 hr, 8 hr, 12 hr, 16 hr and 20 hr in 100mM KH_2PO_4-NaOH (pH 8.0) buffer at 50 ºC. The time-course profile of the surface roughness indicated that longer exposure times with FAST-PETase resulted in higher degree of surface roughness on the pc-PET films. RMS represents root mean square.

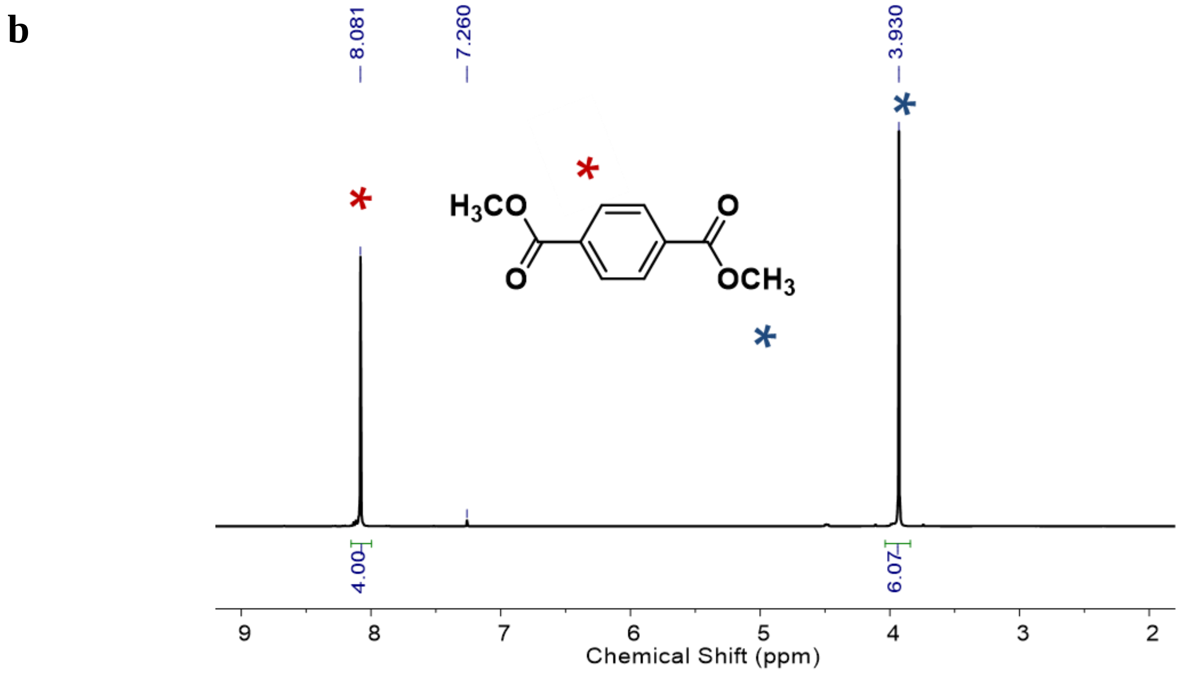


Supplementary Information Fig. 13 | Time-course of PET-hydrolytic activity of LCC and ICCM at reaction temperatures of 55 ºC, 60 ºC, 65 ºC, and 72 ºC. PET-hydrolytic activity was evaluated by measuring the amount of PET monomers (the sum of TPA and MHET) released from hydrolyzing the pc-PET (Bean cake plastic container) film by the tested PHEs at various time points. 100 mM KH_2PO_4-NaOH (pH 8.0) buffer was used for all reactions shown in this figure. All measurement were conducted in triplicate (n=3).

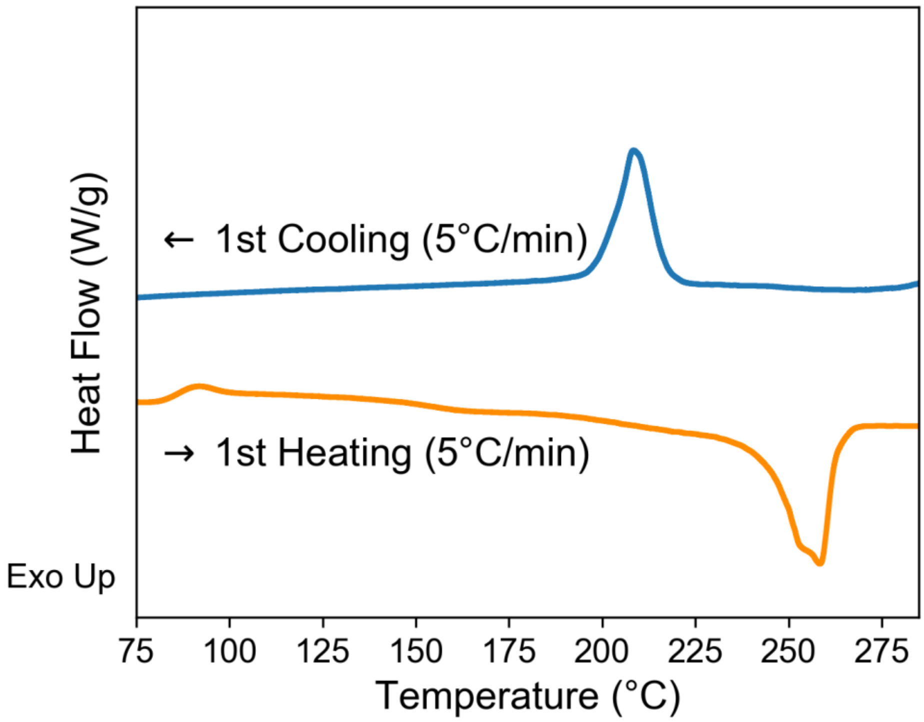


Supplementary Information Fig. 14 | A closed-loop PET recycling process. Demonstration of a closed-loop process for enzymatically degrading and then regenerating PET in the course of several days.

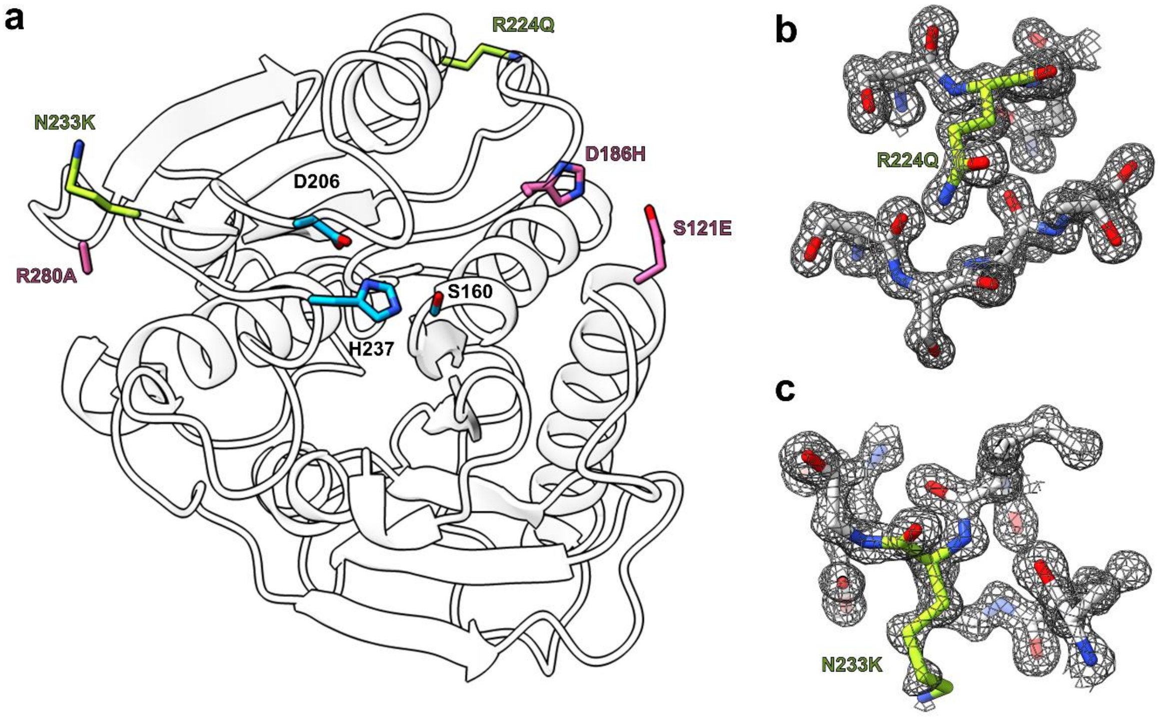




Supplementary Information Fig. 15 | a. ^{1}H NMR (400 MHz, *d*$_6$-DMSO) spectra of TPA recovered from degraded PET solutions. The peak at 8.029 ppm corresponds to the hydrogen nuclei of the benzene ring. **b. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of DMT synthesized from TPA.** The peak at 8.081 ppm corresponds to the hydrogen nuclei of the benzene ring. The peak at 3.93 ppm corresponds to the hydrogen nuclei of the methyl group.



Supplementary Information Fig. 16 | DSC trace of PET regenerated from the degraded solutions. The crystallinity of this regenerated PET is 58.46%. The melting onset is 243.6 °C. The melting peak temperature is 258.4 °C. The glass transition temperature is 84.3 °C.



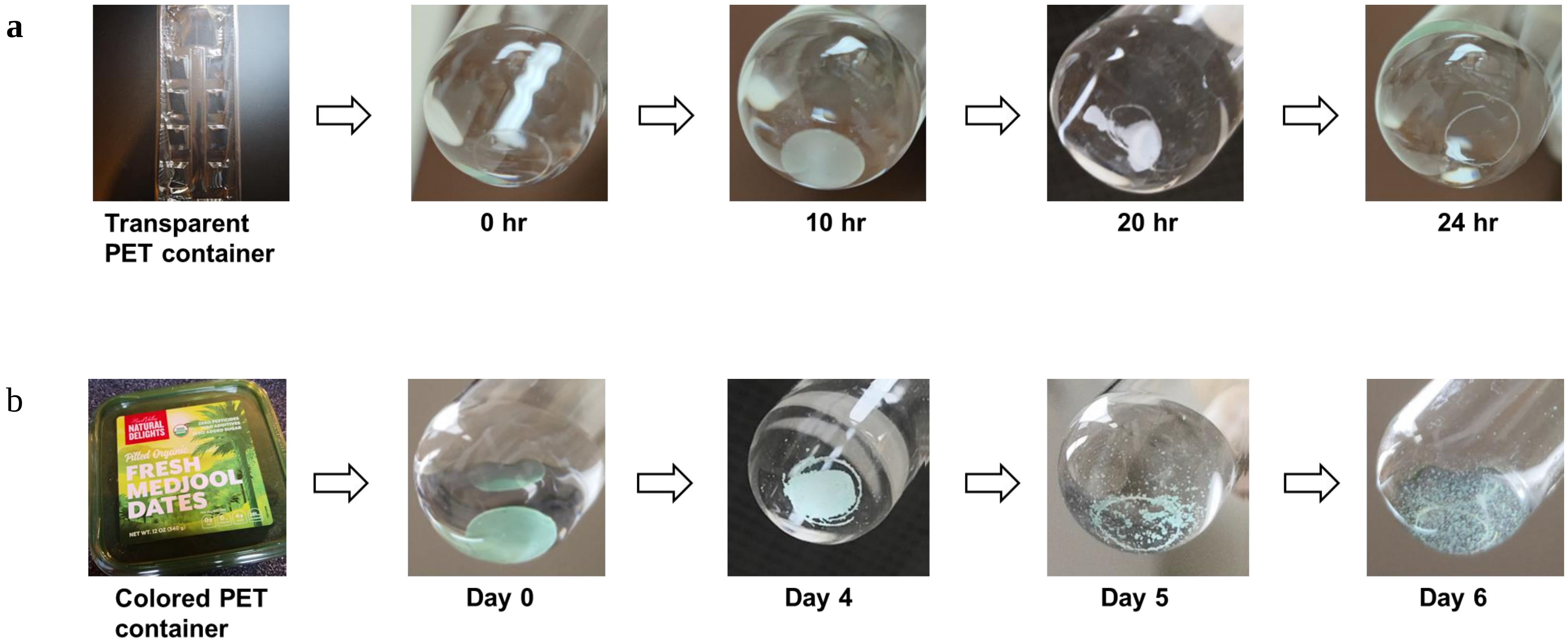
Supplementary Information Fig. 17 | X-ray crystal structure of FAST-PETase. a. Overall crystal structure of FAST-PETase. Catalytic triads (S160, D206, H237) are shown in blue sticks. Mutations originating from ThermoPETase (S121E, D186H, R280A) are shown in pink sticks, and novel mutations predicted by the neural network are shown in green-yellow sticks. **b-c.** $2F_o$-F_c map (contoured at 1.5σ) shown as grey mesh superimposed on the stick models of novel mutation sites (**b.**) R224Q, (**c.**) N233K.

Data collection	
Space group	$P2_12_12_1$
Cell dimensions	
a, b, c (Å)	50.9, 51.2, 84.1
α, β, γ (°)	90.0, 90.0, 90.0
Resolution (Å)	50.00-1.44 (1.46-1.44)*
R_{sym}/ R_{pim}	0.074(0.195)/0.031(0.113)
CC ½ ^{ϒ}	0.988 (0.948)
I / σ	27.4 (3.96)
Completeness (%)	99.4 (94.3)
Redundancy	6.6 (3.5)
Refinement	
Resolution (Å)	43.714 - 1.439 (1.490 - 1.439)
No. reflections	40270 (3753)
R_{work}	0.1515 (0.1641)
$R_{free}^{\pm}$	0.1657 (0.2118)
No. atoms	2344
Protein	1981
Ligand/ion	5
Water	358
B-factors (Å²)	
Protein	7.8
Ligand/ion	17.6
Water	23.2
R.m.s. deviations	
Bond lengths (Å)	0.012
Bond angles (°)	1.18
Ramachandran plot	
Favored	97.68%
Allowed	2.32%
Outliers	0.00%
Molprobity score	1.16 / 97th percentile

*Values for the corresponding parameters in the outermost shell in parenthesis.
$^{ϒ}CC_{1/2}$ is the Pearson correlation coefficient for a random half of the data; the two numbers represent the lowest and highest resolution shell, respectively.
$^{\pm}R_{free}$ is the R_{work} calculated for about 10% of the reflections randomly selected and omitted from refinement.

Supplementary Information Fig. 18 | Statistics of the crystal structural determination of FAST-PETase.

Information about the obtained crystal structure is provided.



Supplementary Information Fig. 19 | Stages of degradation of pc-PET films by FAST-PETase. a. The transparent pc-PET film (6 mm in diameter) was completely degraded (only cutting edges of the film remained) after 24 hrs of a single treatment with FAST-PETase at 50 ^{0}C. b. The colored pc-PET film (6 mm in diameter) was completely degraded (only cutting edges of the film and some colorants remained) after six day of serial treatment with FAST-PETase at 50 ^{0}C. Enzyme (200 nM) treatment was performed with 100 mM KH_2PO_4-NaOH (pH 8.0) buffer.

Reference

1. Narancic, T. *et al.* Genome analysis of the metabolically versatile Pseudomonas umsongensis GO16: the genetic basis for PET monomer upcycling into polyhydroxyalkanoates. *Microb. Biotechnol.* (2021). doi:10.1111/1751-7915.13712

2. Tiso, T. *et al.* Towards bio-upcycling of polyethylene terephthalate. *Metab. Eng.* **66**, 167–178 (2021).

3. Seo, H. *et al.* Production of extracellular PETase from Ideonella sakaiensis using sec-dependent signal peptides in E. coli. *Biochem. Biophys. Res. Commun.* **508**, 250–255 (2019).