

Table S2. Tertiary structure comparison of the full-length cyclomaltodextrinase from *Flavobacterium* sp. No. 92 with representatives of individual GH13 subfamilies.<sup>a</sup>

Subfamily	Enzyme <sup>b</sup>	Source	PDB <sup>c</sup>	C $\alpha$	RMSD
GH13_1	AAMY	<i>Aspergillus oryzae</i>	2TAA	348	1.75
GH13_2	CGT	<i>Bacillus circulans</i>	1CDG	375	1.48
GH13_3	GPMT	<i>Mycobacterium tuberculosis</i>	4U33	330	1.70
GH13_4	AMS	<i>Deinococcus geothermalis</i>	3UCQ	342	1.71
GH13_5	AAMY	<i>Bacillus amyloliquefaciens</i>	3BH4	272	1.77
GH13_6	AAMY	<i>Hordeum vulgare</i>	1HT6	275	1.81
GH13_7	AAMY	<i>Pyrococcus woesei</i>	3QGV	280	1.72
GH13_8	GBE	<i>Homo sapiens</i>	4BZY	320	1.69
GH13_9	GBE	<i>Cyanothece</i> sp. ATCC 51142	5GQU	342	1.62
GH13_10	MOTH	<i>Deinococcus radiodurans</i>	2BHU	319	1.61
GH13_11	ISA	<i>Sulfolobus solfataricus</i>	2VNC	322	1.72
GH13_12	PUL	<i>Streptococcus pneumoniae</i>	2YA0	328	1.62
GH13_13	LDE	<i>Hordeum vulgare</i>	4J3S	325	1.73
GH13_14	PUL	<i>Anoxybacillus</i> sp. LM18-11	3WDH	317	1.76
GH13_15	AAMY	<i>Tenebrio molitor</i>	1CLV	271	1.79
GH13_16	TSY	<i>Mycolicibacterium smegmatis</i>	3ZO9	342	1.58
GH13_17	SUH	<i>Bombyx mori</i>	6LGA	347	1.64
GH13_18	SPH	<i>Bifidobacterium adolscensis</i>	1R7A	304	1.72
GH13_19	M6H	<i>Bacillus halodurans</i>	model (1TCM)	366	1.51
GH13_20	CMMH	<i>Arthrobacter globiformis</i>	5ZXG	361	1.47
GH13_20	CMD	<i>Bacillus</i> sp. I-5	1EA9	370	1.50
GH13_20	NPUL	<i>Geobacillus stearothermophilus</i>	1JOH	365	1.48
GH13_20	GDE	<i>Nostoc punctiforme</i>	2WC7	342	1.42
GH13_20	CMD	<i>Pyrococcus furiosus</i>	4AEF	336	1.37
GH13_20	MGA	<i>Staphylothermus marinus</i>	4AEE	349	1.53
GH13_20	NPUL	<i>Thermoactinomyces vulgaris</i> (TVAIL)	1BVZ	363	1.65
GH13_20	PUL	<i>Thermococcus kodakarensis</i>	5OT1	364	1.46
GH13_20	MGA	<i>Thermus</i> sp. IM6501	1GVI	365	1.52
GH13_21	AAMY	<i>Thermoactinomyces vulgaris</i> (TVAIL)	1UH3	354	1.45
GH13_22	AGS	<i>Cryptococcus neoformans</i>	model (1CYG)	372	1.48
GH13_23	ATGS	<i>Xanthomonas campestris</i>	6AAV	340	1.61
GH13_24	AAMY	<i>Homo sapiens</i>	1HNY	246	1.82
GH13_25	GDE	<i>Candida glabrata</i>	5D06	283	1.90
GH13_26	MOTS	<i>Sacharolobus shibatae</i>	5ZCR	305	1.64
GH13_27	AAMY	<i>Aeromonas hydrophila</i>	model (6M4K)	242	1.85
GH13_28	AAMY	<i>Bacillus subtilis</i>	1BAG	254	1.72
GH13_29	T6PH	<i>Bacillus licheniformis</i>	5BRP	308	1.73
GH13_30	AGLU	<i>Arthrobacter globiformis</i>	model (3ZOA)	332	1.56
GH13_31	ONGLU	<i>Bacillus cereus</i>	1UOK	324	1.66
GH13_32	AAMY	<i>Pseudoalteromonas haloplanktis</i>	1AQH	240	1.68
GH13_33	TSY	<i>Pseudomonas stutzeri</i>	model (6LI9)	327	1.69
GH13_34	4F2hc	<i>Homo sapiens</i>	2DH2	290	1.66
GH13_35	rBAT	<i>Homo sapiens</i>	6LI9	342	1.74
GH13_36	AAMY	<i>Bacteroides thetaiotaomicron</i>	3K8K	336	1.52
GH13_37	AAMY	uncultured bacterium	5H05	343	1.60
GH13_38	AGLU	<i>Bacteroides cellulosilyticus</i>	model (1JIB)	353	1.50
GH13_39	APUL	<i>Alicyclobacillus acidocalarius</i>	model (2D0G)	355	1.45

GH13_40	AGLU	<i>Sacharomyces cerevisiae</i>	3A47	308	1.83
GH13_41	AAMY	<i>Eubacterium rectale</i>	model (2YA1)	310	1.64
GH13_42	M6H	<i>Microbacterium aurum</i>	model (1QHO)	362	1.50
GH13_43	AAMY	<i>Haloarcula hispanica</i>	model (1TCM)	311	1.53
GH13_44	AGLU	Bifidobacteriaceae bacterium	model (3ZOA)	331	1.56
GH13_45	AAMY	<i>Geobacillus thermoleovorans</i>	4E2O	381	1.52
GH13_45	NSA	<i>Bacillus megaterium</i>	model (4E2O)	364	1.54

<sup>a</sup> Results of superposition of the full-length cyclomaltodextrinase from *Flavobacterium* sp. No. 92 ([24]; PDB code: 1H3G) with representatives from individual GH13 subfamilies are shown as the number of corresponding C $\alpha$  atoms and the RMSD value in Å (the last two columns).

<sup>b</sup> The individual enzymes are abbreviated as follows: AAMY,  $\alpha$ -amylase; CGT, cyclodextrin glucanotransferase; GPMT,  $\alpha$ -1,4-glucan: phosphate  $\alpha$ -maltosyltransferase; AMS, amylosucrase; GBE,  $\alpha$ -glucan branching enzyme; MOTH, maltooligosyltrehalose trehalohydrolase; ISA, isoamylase; PUL, pullulanase; LDE, limit dextrinase; TSY, trehalose synthase; SUH, sucrose hydrolase; SPH, sucrose phosphorylase; M6H, maltohexaose-producing amylase; CMMH, cyclic maltosyl-maltose hydrolase; CMD, cyclomaltodextrinase; NPUL, neopullulanase; GDE, glycogen debranching enzyme; MGA, maltogenic amylase; AGS,  $\alpha$ -1,3-glucan synthase; ATGS,  $\alpha$ -transglucosidase; MOTS, maltooligosyltrehalose trehalosynthase; T6PH, trehalose-6-phosphate hydrolase; AGLU,  $\alpha$ -glucosidase; OGLU, oligo-1,6-glucosidase; 4F2hc, 4F2 heavy-chain antigen; rBAT, amino acid transport protein rBAT; APUL, amylopullulanase; NSA, non-specified amylase.

<sup>c</sup> PDB codes from the Protein Data Bank (if available); for models, the PDB code of a template PDB is shown in parenthesis.