

C. Module 3

104Y_A beta-agarase A (E.C.3.2.1.81); BETA-AGARASE, GLYCOSIDE HYDROLASE FAMILY 16; HET: SO4; 1.48A (Zobellia galactanivorans) SCOP: b.29.1.2; Related PDB entries: 1URX_A ; Related PDB entries: 1URX_A
Probability: 81.76%, E-value: 69, Score: 29.46, Aligned cols: 188, Identities: 16%, Similarity: 0.189

Table with 5 columns: Query ID (Q ss_pred, Q WP_009778041, Q Consensus), Target ID (T Consensus, T 104Y_A, T ss_dssp, T ss_pred), Alignment (sequence and secondary structure), and Scores (e.g., 80 (340), 158 (340), 213 (288)).

Supplementary figure 1. Results of the HHpred search seeded with the multiple sequence alignments prepared from proteins in module 1 (A), 2 (B) and 3 (C). H(h), α-helix; C(c), coil; Q, query; T, target; ss, secondary structure.

Multiple sequence alignment of GH16 family proteins and their inactive derivatives. The table lists sequences from various bacterial and viral sources, including Pseudomonas carriagevenora, Bacillus licheniformis, and Mimivirus. Sequences are numbered on the left and right, indicating specific residues. Active proteins are shown in red text, while inactive derivatives are shown in green text. Inactive sequences are indicated with their corresponding PDB identifiers in parentheses. Conserved residues are shown in bold. Some sequences are truncated with ellipses. The alignment is presented in two columns, with the first column containing sequences 1-332 and the second column containing sequences 112-950.

Supplementary figure 2. Multiple sequence alignment of GH16 family proteins and their inactive derivatives. Enzymatically active GH16 family proteins for which X-ray structures available are shown in red and indicated with the corresponding PDB identifiers. Inactivated GH16 derivatives encoded by diverse bacteria and giant viruses are indicated with green and red fonts, respectively. Note that bacterial sequences include representatives of all 3 modules defined in Figure 2A. Long, non-conserved insertions are not shown for clarity, with the exact number of omitted residues indicated in parenthesis.

Supplementary table 1. Composition of the Modules 1 to 3.

Accession #	Organism name	Taxon
Module 1		
WP_004001160	<i>Streptomyces viridochromogenes</i>	Actinobacteria
WP_013422495	<i>Frankia inefficax</i>	Actinobacteria
WP_018542795	unclassified <i>Streptomyces</i>	Actinobacteria
WP_019070481	<i>Streptomyces hokutonensis</i>	Actinobacteria
WP_019524852	unclassified <i>Streptomyces</i>	Actinobacteria
WP_019524853	unclassified <i>Streptomyces</i>	Actinobacteria
WP_033294507	<i>Amycolatopsis jejuensis</i>	Actinobacteria
WP_036346721	<i>Micromonospora</i>	Actinobacteria
WP_043667143	<i>Streptomyces xylophagus</i>	Actinobacteria
WP_051763122	<i>Streptomyces virginiae</i>	Actinobacteria
WP_051773929	<i>Streptomyces</i> sp. NRRL S-237	Actinobacteria
WP_051782626	unclassified <i>Streptomyces</i>	Actinobacteria
WP_051816291	<i>Streptomyces</i> sp. NRRL WC-3744	Actinobacteria
WP_051818725	<i>Streptomyces</i>	Actinobacteria
WP_051848524	<i>Streptomyces</i> sp. NRRL WC-3725	Actinobacteria
WP_051854226	unclassified <i>Streptomyces</i>	Actinobacteria
WP_052021393	<i>Actinokineospora spheciospongiae</i>	Actinobacteria
WP_052183290	<i>Streptomyces</i> sp. UNC401CLCol	Actinobacteria
WP_052681576	<i>Saccharothrix</i> sp. ST-888	Actinobacteria
WP_053211603	<i>Streptomyces antibioticus</i>	Actinobacteria
WP_055613714	<i>Streptomyces phaeochromogenes</i>	Actinobacteria
WP_055613717	<i>Streptomyces phaeochromogenes</i>	Actinobacteria
WP_066927533	<i>Streptomyces</i> sp. NBRC 110611	Actinobacteria
WP_073215198	<i>Streptomyces</i> sp. NBRC 110465	Actinobacteria
WP_073496364	<i>Streptomyces phaeoluteigriseus</i>	Actinobacteria
WP_073904122	<i>Streptomyces</i> sp. CB02009	Actinobacteria
WP_078637708	<i>Streptomyces</i>	Actinobacteria
WP_079134226	unclassified <i>Streptomyces</i>	Actinobacteria
WP_079134227	unclassified <i>Streptomyces</i>	Actinobacteria
WP_079141677	<i>Streptomyces</i> sp. LUP30	Actinobacteria
WP_079149609	<i>Streptomyces</i> sp. EN27	Actinobacteria
WP_079180745	<i>Streptomyces</i> sp. CB02058	Actinobacteria
WP_079180747	<i>Streptomyces</i> sp. CB02058	Actinobacteria
WP_079185489	<i>Streptomyces</i> sp. NBRC 110465	Actinobacteria
WP_079188286	<i>Streptomyces</i> sp. CB0200	Actinobacteria
WP_079192651	<i>Streptomyces</i> sp. CB01883	Actinobacteria
WP_083753708	<i>Actinosynnema</i> sp. ALI-1.44	Actinobacteria
WP_087924989	<i>Streptomyces albireticuli</i>] 134	Actinobacteria
WP_088961757	<i>Micromonospora purpureochromogenes</i>	Actinobacteria
WP_091451464	<i>Alloactinosynnema iranicum</i>	Actinobacteria
WP_092650511	<i>Actinopolymorpha singaporensis</i>	Actinobacteria
WP_092886397	<i>Actinopolymorpha cephalotaxi</i>	Actinobacteria
WP_093471991	unclassified <i>Streptomyces</i>	Actinobacteria
WP_093627747	<i>Streptomyces</i> sp. 3213.3	Actinobacteria

WP_093736433	unclassified Streptomyces	Actinobacteria
WP_093908613	Streptomyces sp. Cf386	Actinobacteria
WP_095578871	Streptomyces albireticuli	Actinobacteria
WP_100825925	Streptomyces sp. 69	Actinobacteria
WP_106246877	Allonocardia opalescens	Actinobacteria
WP_106432501	unclassified Streptomyces	Actinobacteria
WP_107072723	Streptomyces sp. NRRL B-1568	Actinobacteria
WP_109497567	Streptomyces sp. Act143	Actinobacteria
WP_110079847	Actinokineospora mزابensis	Actinobacteria
WP_116021934	Actinomadura umbrina	Actinobacteria
WP_116021939	Actinomadura umbrina	Actinobacteria
WP_116180669	Kutzneria buriramensis	Actinobacteria
WP_121801026	Streptomyces griseocarneus	Actinobacteria
WP_123440892	Streptomyces sp. PanSC9	Actinobacteria
WP_125594626	Streptomyces sp. WAC07061	Actinobacteria
WP_125814831	Streptomyces sp. WAC07149	Actinobacteria
WP_129593328	Streptomyces sp. C	Actinobacteria
WP_130876631	Streptomyces netropsis	Actinobacteria
WP_138043881	Streptomyces sp. NEAU-C151	Actinobacteria
WP_141208225	Streptomyces griseorubiginosus	Actinobacteria
WP_141561871	Micromonospora sp. WMMA1996	Actinobacteria
WP_141684583	Micromonospora sediminicola	Actinobacteria
WP_143593014	Streptomyces albireticuli	Actinobacteria
WP_145788523	Kitasatospora atroaurantiaca	Actinobacteria
WP_146045455	Streptomyces eurocidicus	Actinobacteria
WP_146238386	Streptomyces sp. Act143	Actinobacteria
WP_146238387	Streptomyces sp. Act143	Actinobacteria
WP_147472096	Streptomyces griseocarneus	Actinobacteria
WP_148349770	Actinomadura syzygii	Actinobacteria
WP_148349773	Actinomadura syzygii	Actinobacteria
WP_148767260	Actinomadura sp. CYP1-5	Actinobacteria
WP_148767263	Actinomadura sp. CYP1-5	Actinobacteria
WP_153278161	Saccharothrix syringae	Actinobacteria
WP_153541889	Streptomyces sp. RB17	Actinobacteria
WP_154936519	Micromonospora palomenae	Actinobacteria
WP_154936522	Micromonospora palomenae	Actinobacteria
WP_157745954	Micromonospora purpureochromogenes	Actinobacteria
WP_159042716	Streptomyces curacoii	Actinobacteria
WP_159395205	Streptomyces albireticuli	Actinobacteria
WP_161069931	Streptomyces sp. HUCO-GS316	Actinobacteria
WP_161108180	Streptomyces sp. XHT-2	Actinobacteria
WP_161108181	Streptomyces sp. XHT-2	Actinobacteria
WP_161231499	Streptomyces sp. SID4956	Actinobacteria
WP_161241892	Streptomyces sp. SID2888	Actinobacteria
WP_161241895	Streptomyces sp. SID2888	Actinobacteria
WP_161241896	Streptomyces sp. SID2888	Actinobacteria
WP_161290971	Streptomyces sp. SID1046	Actinobacteria

WP_168211442	Actinosynnema sp. ALI-1.44	Actinobacteria
WP_053601342	Bacillus sp. FJAT-18017	Firmicutes
WP_066204414	Bacillus sp. FJAT-27225	Firmicutes
WP_099355020	Bacillus onubensis	Firmicutes
WP_099364288	Bacillus onubensis	Firmicutes
WP_011952500	Sphingomonas wittichii	Proteobacteria
WP_016746823	Sphingomonas wittichii	Proteobacteria
WP_047168197	Sphingomonas sp. Y57	Proteobacteria
WP_052420046	Hyalangium minutum	Proteobacteria
WP_056354592	unclassified Sphingomonas	Proteobacteria
WP_132145912	Luteibacter rhizovincinus	Proteobacteria
WP_146728083	Minicystis rosea	Proteobacteria
WP_170328229	Ruegeria arenilitoris	Proteobacteria
WP_170609244	Ruegeria conchae	Proteobacteria

Module 2

WP_068013487	Nocardia mexicana	Actinobacteria
WP_024802787	Nocardia sp. BMG51109	Actinobacteria
WP_146251404	Nocardia tenerifensis	Actinobacteria
WP_138666465	Nonomuraea turkmeniaca	Actinobacteria
WP_028931974	Pseudonocardia asaccharolytica	Actinobacteria
WP_009478479	Rhodococcus sp. JVH1	Actinobacteria
WP_055722186	Streptomyces	Actinobacteria
WP_050371984	Streptomyces acidiscabies	Actinobacteria
WP_075730970	Streptomyces acidiscabies	Actinobacteria
WP_053210749	Streptomyces antibioticus	Actinobacteria
WP_037701643	Streptomyces atratus	Actinobacteria
WP_062050432	Streptomyces canus	Actinobacteria
WP_050782599	Streptomyces griseoflavus	Actinobacteria
WP_073502273	Streptomyces paucisporeus	Actinobacteria
WP_100203414	Streptomyces sp. TRM SA0054	Actinobacteria
WP_018839510	unclassified Streptomyces	Actinobacteria
WP_098503344	Thermoflexus hugenholtzii	Chloroflexi
WP_151729905	Thermogemmatispora aurantia	Chloroflexi
WP_066289961	Fictibacillus arsenicus	Firmicutes
WP_066394060	Fictibacillus phosphorivorans	Firmicutes
WP_019637377	Paenibacillus fonticola	Firmicutes
WP_144873436	Paenibacillus ihbetae	Firmicutes
WP_127588546	Paenibacillus koleovorans	Firmicutes
WP_076287080	Paenibacillus odorifer	Firmicutes
WP_091167356	Paenibacillus sp. 1_12	Firmicutes
WP_053375461	Paenibacillus sp. FJAT-27812	Firmicutes
WP_039879466	Paenibacillus sp. FSL R7-0273	Firmicutes
WP_036692278	Paenibacillus sp. FSL R7-269	Firmicutes
WP_129437925	Paenibacillus sp. FW100M-2	Firmicutes
WP_057314481	Paenibacillus sp. Soil766	Firmicutes
WP_150270317	Paenibacillus sp. SYSU G01001	Firmicutes

WP_038699482	Paenibacillus stellifer	Firmicutes
WP_093338107	Salibacterium halotolerans	Firmicutes
WP_006159786	Cupriavidus basilensis	Proteobacteria
WP_013954189	Cupriavidus necator	Proteobacteria
WP_013954198	Cupriavidus necator	Proteobacteria
WP_116263445	Pseudomonas sp. OV081	Proteobacteria

Module 3

WP_009778041	Janibacter sp. HTCC2649	Actinobacteria
WP_091356076	Frankineae bacterium MT45	Actinobacteria
WP_096304281	Jatrophihabitans sp. GAS493	Actinobacteria
WP_135839310	Nocardioides sp. MMS17-SY213	Actinobacteria
WP_139131788	Micromonospora chersina	Actinobacteria
WP_141844292	Humibacillus xanthopallidus	Actinobacteria
WP_148616077	Nocardioides rubriscoriae	Actinobacteria
WP_151461420	Micromonospora sp. AMSO31t	Actinobacteria
WP_124897093	Haloplanus aerogenes	Halobacteria
WP_056193950	Pelomonas sp. Root1237	Proteobacteria
WP_056264676	unclassified Pelomonas	Proteobacteria
WP_057300625	Pelomonas sp. Root1217	Proteobacteria
WP_100922660	Candidatus Thiodictyon syntrophicum	Proteobacteria