

Supplementary material

Bacillus subtilis lipase A – lipase or esterase?

Paula Bracco ¹, Nelleke van Midden ¹, Epifanía Arango ¹, Guzman Torrelo ¹, Valerio Ferrario ², Lucia Gardossi ² and Ulf Hanefeld ^{1,*}

¹ Biokatalyse, Afdeling Biotechnologie, Technische Universiteit Delft, Van der Maasweg 9, 2629 HZ Delft, The Netherlands; paulabracco@gmail.com (P.B.); nellekevanmidden@gmail.com (N.v.M.); epifaniarango@gmail.com (E.A.); guzman.torrelo@hotmail.com (G.T.);

² Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste, Via Licio Giorgieri 1, 34127 Trieste, Italy; valerio.ferrario@gmail.com (V.F.); gardossi@units.it (L.G.)

* Correspondence: u.hanefeld@tudelft.nl; Tel.: +31-15-278-9304 (U.H.)

BIO GPS descriptors

Table S1 Enzymes utilized for the Bio GPS study with the relevant PDB codes.

Enzyme class	PDB code	Source	Enzyme class	PDB code	Source
Lipases	1CRL	<i>Candida rugosa</i>	Proteases	1GVK	<i>Sus scrofa</i>
	1DTE	<i>Humicola lanuginosa</i>		1NPM	<i>Mus musculus</i>
	1ETH	<i>Sus scrofa</i>		1PPB	<i>Homo sapiens</i>
	1EX9	<i>Pseudomonas aeruginosa</i>		1QFM	<i>Sus scrofa</i>
	1GPL	<i>Cavia Porcellus</i>		1TAW	<i>Bos Taurus</i>
	1K8Q	<i>Canis lupus familiaris</i>		1TM1	<i>Bacillus amyloliquefaciens</i>
	1LPB	<i>Homo sapiens</i>		1YU6	<i>Bacillus licheniformis</i>
	1TCA	<i>Candida antarctica</i>		2XE4	<i>Leshmania major</i>
	2FX5	<i>Pseudomonas mendocina</i>		3F7O	<i>Peacelomyces lilacinus</i>
	2NW6	<i>Burkholderia cepacia</i>			
2W22	<i>Geobacillus thermocatenulatus</i>				
Esterases	1AUO	<i>Pseudomonas fluorescens</i>	1A2W	<i>Xantomonas campestris</i>	
	1BS9	<i>Penicillium purpurogenum</i>	1GM9	<i>Escherichia coli</i>	
	1C7J	<i>Bacillus subtilis</i>	1HL7	<i>Microbacterium sp</i>	
	1CLE	<i>Candida cylindracea</i>	1M21	<i>Stenotrophomonas maltophilia</i>	
	1JU3	<i>Rhodococcus sp.</i>	1MPL	<i>Streptomyces sp.</i>	
	1QOZ	<i>Tricoderma reesei</i>	1MUO	<i>Thermoplasma acidophilum</i>	
	1USW	<i>Aspergillus niger</i>	1QTR	<i>Serratia marcescens</i>	
	2ACE	<i>Torpedo californica</i>	3A2P	<i>Arthrobacter sp.</i>	
	2WFL	<i>Rauvolfia serpentine</i>	3K3W	<i>Alcaligenes faecalis</i>	
	3KVN	<i>Pseudomonas aeruginosa</i>	3K84	<i>Rattus norvegicus</i>	
		3NWO	<i>Mycobacterium smegmatis</i>		

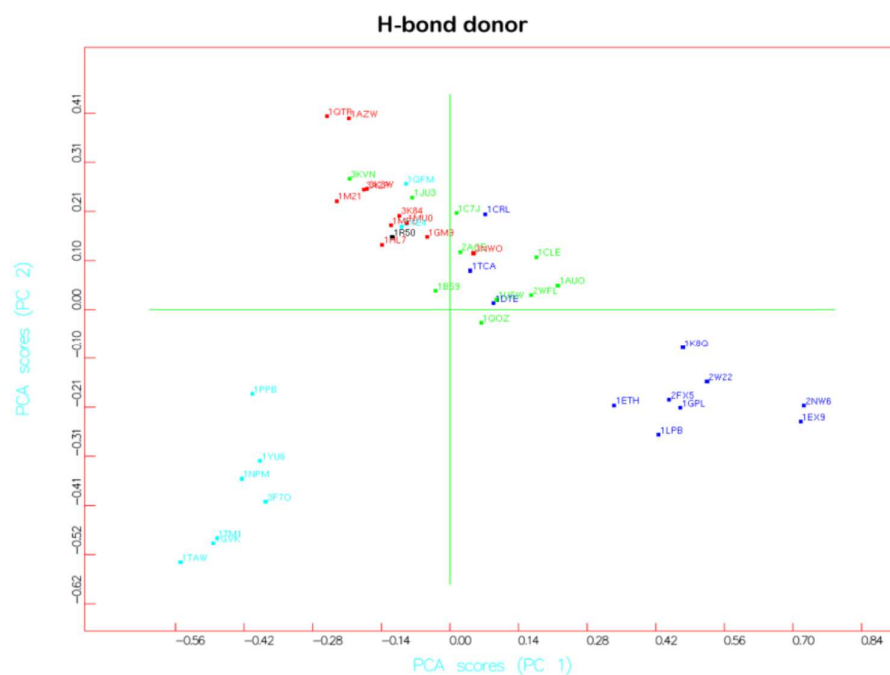


Figure S1a

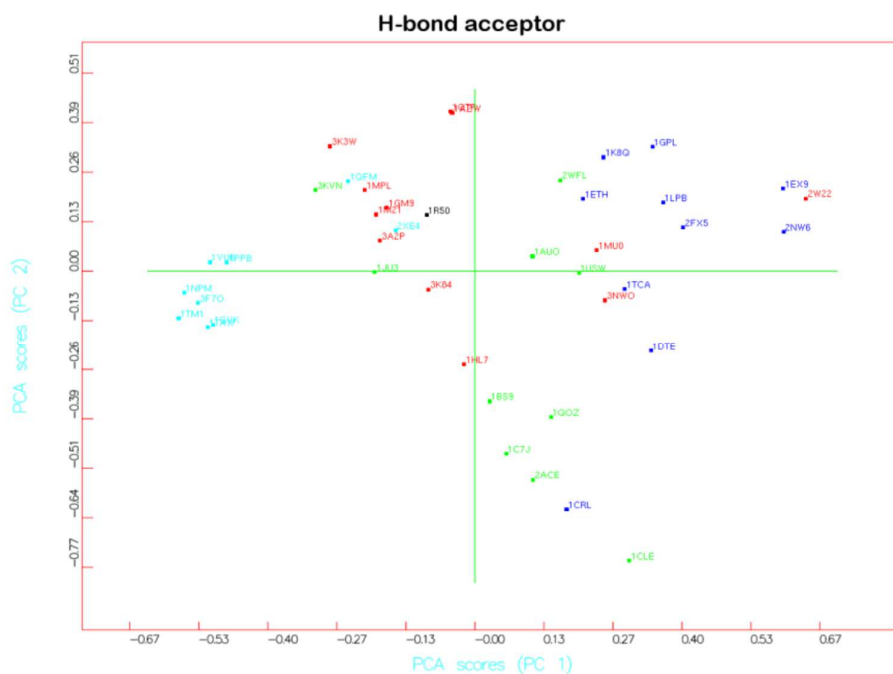


Figure S1b

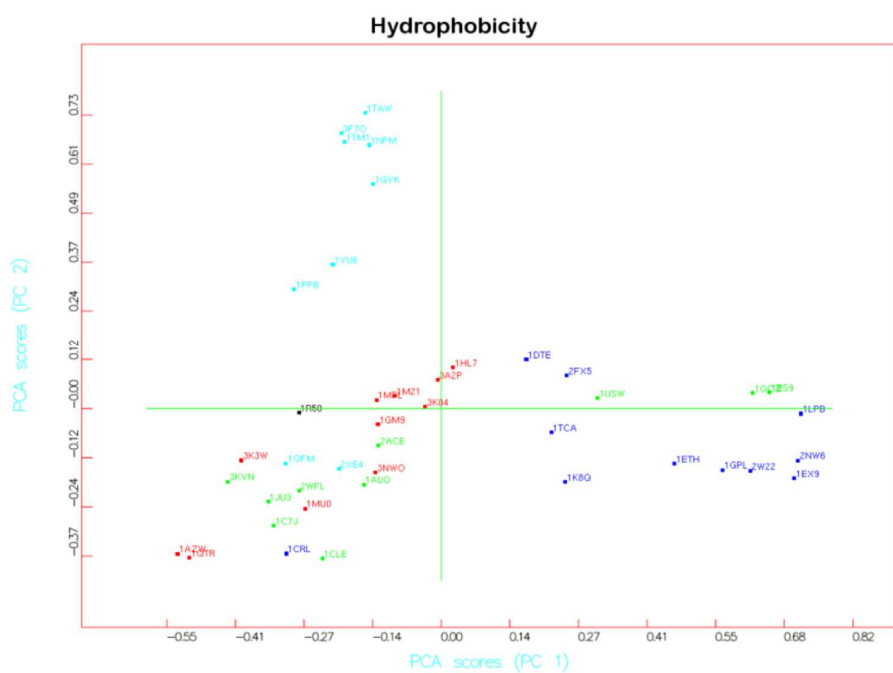


Figure S1c

Figure S1. Bio GPS of 43 serine hydrolases, for BSLA the data of pdb 1R50 were utilized: (a) H-bond donor; (b) H-bond acceptor; (c) Hydrophobicity. The PDB codes of the processed enzyme structures are indicated in different colors according to their class: lipases in blue, amidases in red, proteases in cyan and esterases in green; the BSLA structure is in black.