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The Synthetic Potential of Fungal Feruloyl Esterases: a Correlation with Current Classification Systems and Predicted Structural Properties

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Received: 21 May 2018; Accepted: 1 June 2018; Published: 7 June 2018

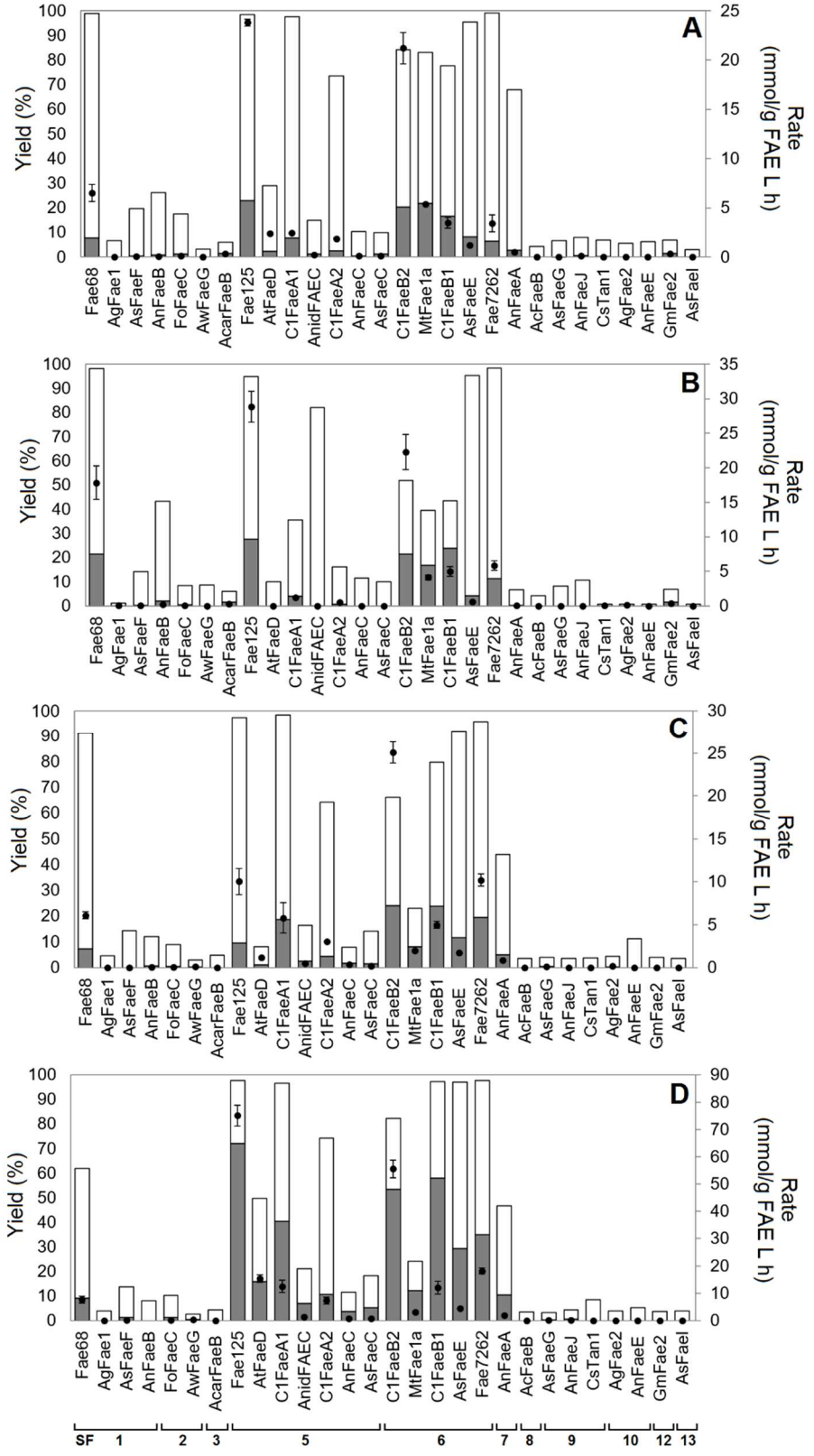

Figure S1. Synthesis of (A) PFA (B) PCA (C) BFA and (D) GFA. Reaction conditions: 50 mM donor (VFA or VCA), 200 mM acceptor, 0.2 mg protein mL^{-1}, 53.4: 43.4: 3.2 v/v/v *n*-hexane: *t*-butanol: buffer, 45°C, no agitation, 24 h of incubation. Grey column: transesterification yield; White column: hydrolysis yield; Black circle: Specific rate of transesterification. The error bars represent the standard deviation between two duplicates.

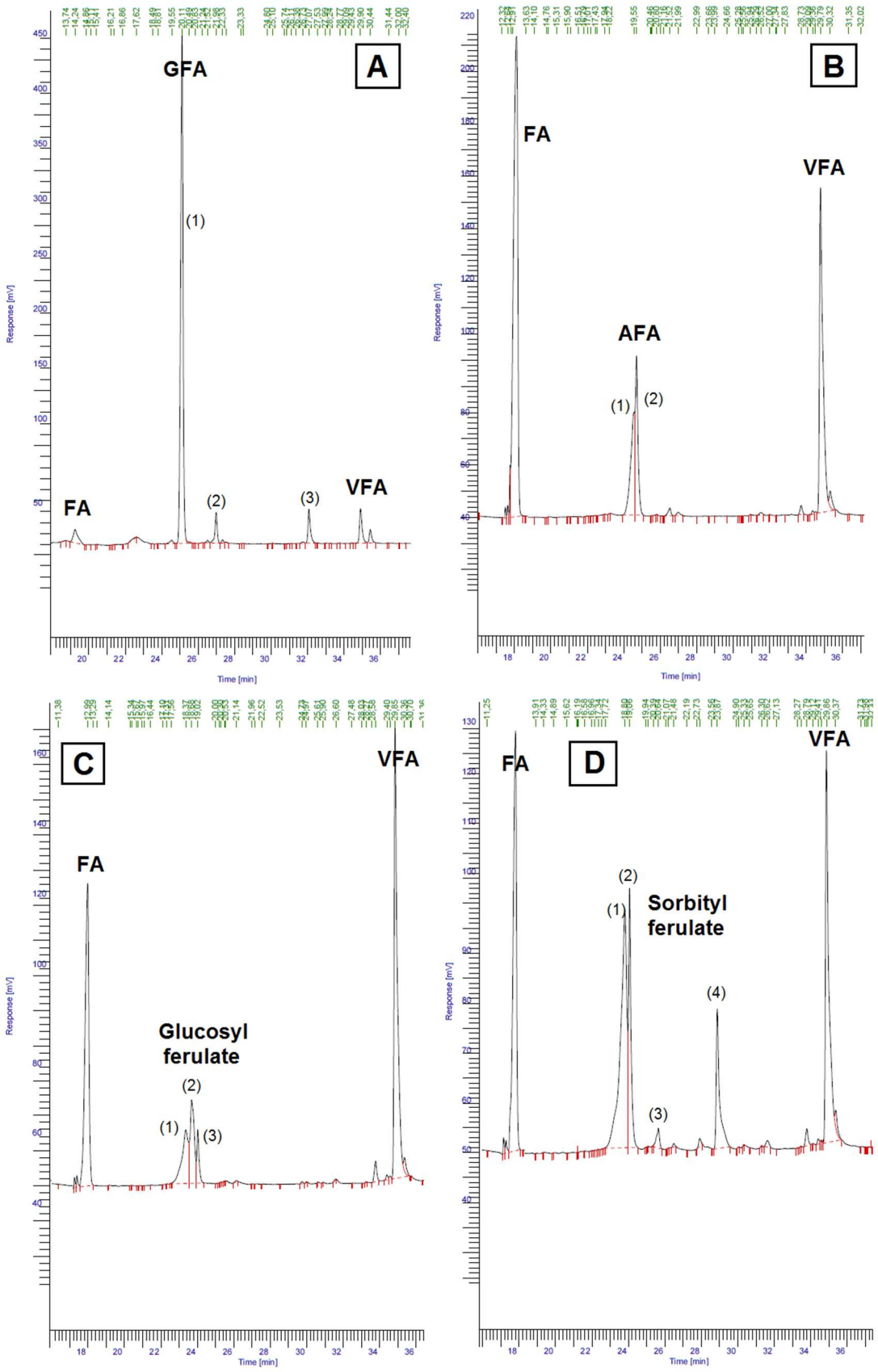

Figure S2. HPLC chromatograms for (A) GFA (B) AFA (C) Glycosyl ferulate and (D) Sorbityl ferulate synthesis.

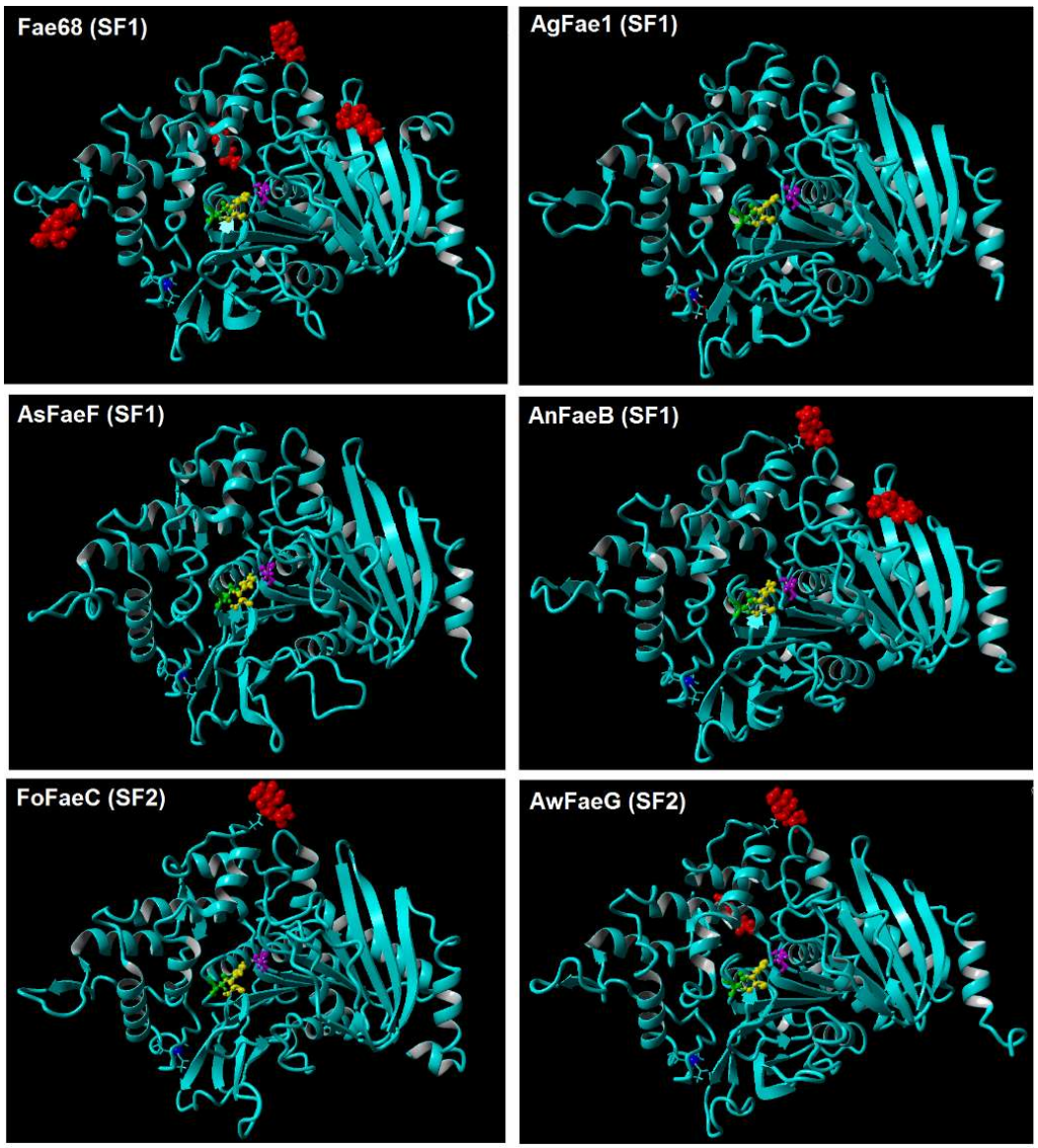

Figure S3. Predicted structures for SF1-2 FAEs obtained by homology modeling using YASARA Structure (YASARA Biosciences GmbH, Vienna, Austria). Magenta: Catalytic serine; Yellow: Catalytic Histidine; Green: Catalytic Aspartate; Red: Predicted glycosylation; Blue: Ca^{+2}.

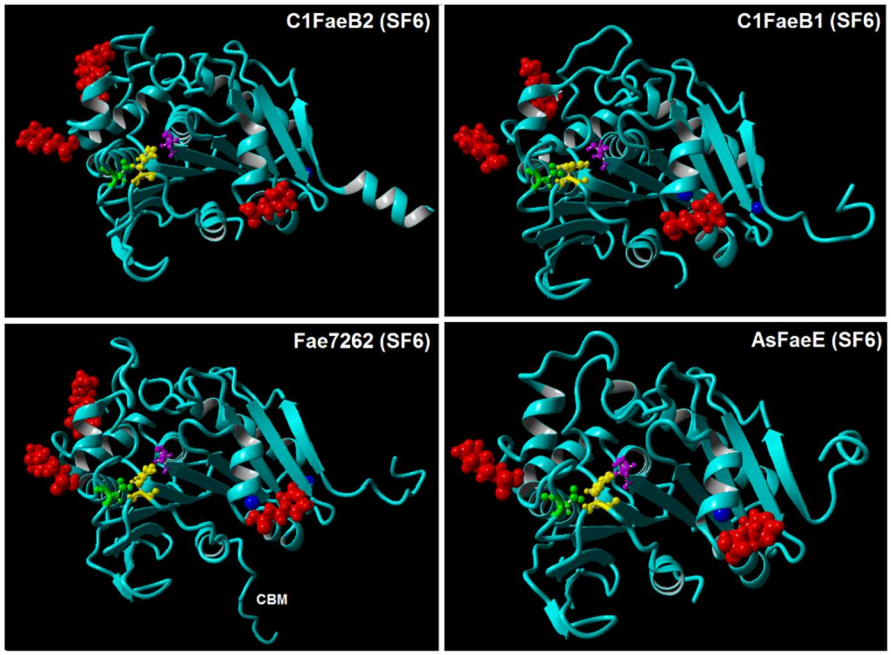

Figure S4. Predicted structures for SF6 FAEs obtained by homology modeling using YASARA Structure (YASARA Biosciences GmbH, Vienna, Austria). Magenta: Catalytic serine; Yellow: Catalytic Histidine; Green: Catalytic Aspartate; Red: Predicted glycosylation; Blue: Na^+.

Table S1. Structure templates and quality test results on best fully refined models exported by YASARA Structure for selected fungal FAEs (SF1-2 and SF6).

SF	Enzyme	Template (PDB ID)	Seq. Identity (%)	Oligo-state	Seq. Similarity	Range	Coverage	Description	Z-score[a]			
									Dihedrals	Packing 1D	Packing 3D	Overall
1	Fae68	AoFaeB from *Aspergillus oryzae* (3WMT_A)	69.14	Homo-dimer	0.53	41 - 556	0.90	Probable feruloyl esterase B-1	0.426 Optimal	-0.411 Good	-1.496 Satisfactory	-0.794 Good
	AgFae1		59.56		0.49	22 - 526	0.95		0.341 Optimal	-0.521 Good	-1.514 Satisfactory	-1.858 Good
	AsFaeF		56.00		0.48	23 - 526	0.95		0.195 Optimal	-0.591 Good	-1.612 Satisfactory	-0.952 Good
	AnFaeB		52.71		0.47	22 - 521	0.96		0.392 Optimal	-0.603 Good	-1.629 Satisfactory	-0.936 Good
2	FoFaeC		49.70		0.46	2 - 503	0.98		0.122 Optimal	-0.768 Good	-1.704 Satisfactory	-1.074 Satisfactory
	AwFaeG		53.71		0.46	26 - 530	0.94		0.321 Optimal	-0.661 Good	-1.591 Satisfactory	-0.951 Good
6	C1FaeB2	Acetyl xylan esterase from *Aspergillus awamori* (5X6S)	42.96	Homo-dimer	0.43	19 - 290	0.93	Acetyl xylan esterase A	-0.304 Optimal	-0.820 Good	-1.630 Satisfactory	-1.034 Satisfactory
	C1FaeB1		41.64		0.43	21 - 292	0.91		0.385 Optimal	-0.740 Good	-1.804 Satisfactory	-1.071 Satisfactory
	AsFaeE		45.32		0.44	20 - 292	0.91		0.206 Optimal	-1.495 Good	-1.495 Satisfactory	-0.858 Good
	Fae7262		45.11		0.43	23 - 291	0.75		0.080 Optimal	-0.578 Good	-1.984 Satisfactory	-1.137 Satisfactory

[a]: Bad (-4 to -3) Optimal (0 to 4).