



STRUCTURAL
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Supporting information for article:

The structure of *Phocaeicola vulgatus* sialic acid acetylcetase

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Table S1 Structurally homologous enzymes to the PvSAE Apo I structure, identified using the DALI server (Holm, 2020).

Description	Source	PBD	Z score	RMSD / Å	L-align	Identity / %
Putative platelet activating factor	<i>Streptococcus pneumonia</i>	2hsj	27.4	1.7	194	28
GDSL-like lipase	<i>Parabacteroides distasonis</i>	3p94	24.7	2.0	183	25
Putative acylhydrolase	<i>Bacteroides fragilis</i>	4ppy	24.2	2.4	190	26
GDSL-like protein	<i>Bacteroides uniformis</i>	4iyj	24.2	2.4	190	26
Brain platelet-activating factor acetylhydrolase	<i>Bos taurus</i>	3dt9	22.3	2.1	185	20

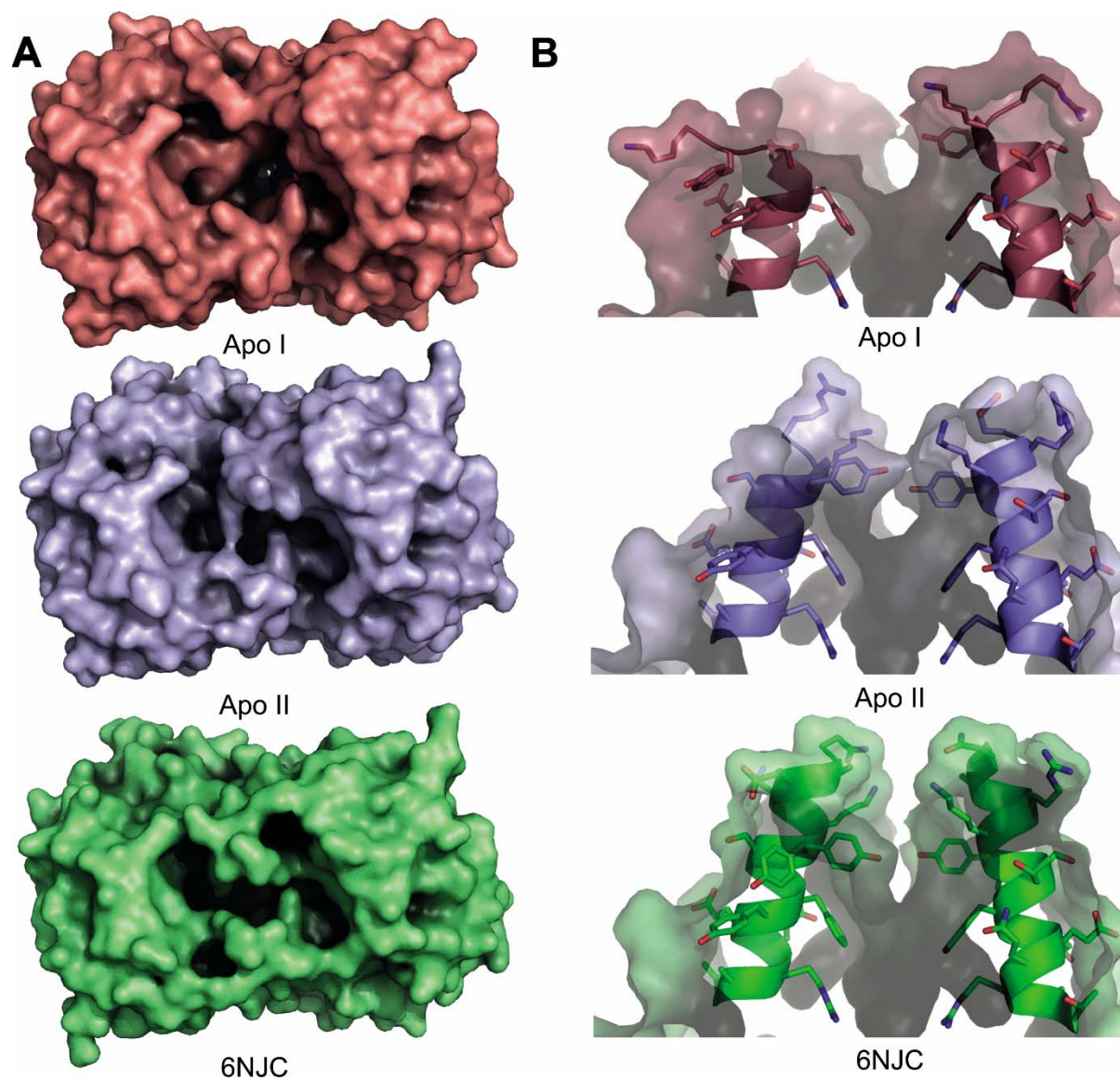


Figure S1 Conformational changes of the N-terminal α -helix. **A)** Surface representation of the Apo I, Apo II and 6njc structures as viewed from above the active site. **B)** The side view of the N-terminal helix from the same structures with residues present in the helix shown in stick representation.

PvSAE	1	-----
BfEstA	1	-----
pAF-AH	1	-----
EcNanS	1	MGSSHHHHHHSNAIISPDYYYVLTVAGQSNAMAYGEGPLPDREDAPHPRIKQLARFAH
		Block I
PvSAE	1	-----ERKYSTFYEQRATLFEELPVTSKDIIFL*GNSITNGCE--
BfEstA	1	--MKKIFFLVVILTLSELLCRAQERKYSTFYQYQYRATLFEELPVTSSDIIFL*GNSITNGAE--
pAF-AH	1	--MSGDENPASKPTPVQDVQGDGRWMSLHHRFVADSKDKPE---EVVFI*GDSLVLQLMHQ
EcNanS	61	THPGGPSCHFNDIIP*LTHCPHDVQDMQSYHHPLATNHQTQYGT*VVGQALHIARKLLPFIPD
		Block II
		Block III
PvSAE	38	---WAELFQNKNVKNR*GISGDI*CMGVYDRLD--PIVKGKPAKIFLLI*GINDVSRGTSADK
BfEstA	58	---WAELFKNKHVKNR*GISGDI*CMGVYDRLD--AILKGGKPAKIFLLI*GINDVSRGTPADT
pAF-AH	55	SEIWRLEFSPLHALNF*GI*GGDSTQHV*LVWRLENGELEHIRPKIVV*VW*GTNNH--GHTAEQ
EcNanS	121	-----NAGILIVPCCRGGSAFT---AGSEGTYSERHGASHDACRWGTDTP
PvSAE	93	IISEISMIVRKIKQESPKTKLYLQSVLPVND*CYGMFN*GHTSRWQV*VQ*INDLL-EPLAV-
BfEstA	113	I*VSRIEMIVRKIKADSPKTKLYLQSVLPVTDHYNMFKGHTSHWQV*IP*EINKGL-VGLAE-
pAF-AH	113	VTGGIKAI*VQLVNERQPQARVV*VGL*LLPRGQH-----PNPLREKNRRV*NELVRAALAG-
EcNanS	163	LYQDLVSRTRAALVKNPQNK-FLGVCWMQGE*FDLM*TSDYASHPQHFNHMV*EAFRRDLKQY
		Block V
PvSAE	151	KEGVAYIDLYSHFVEKETGKMNPVYTND*GLHLL*GKGYLLWRDIVKPYVDQK-----
BfEstA	171	KEGATYIDLYSHFIDKQ*TGKMNTTYTND*GLHLL*GKGYLKWVEIVKPYIGKK-----
pAF-AH	166	HPRAHFLDADPGFVHSD-GTIS*HDMYD*YLLHLSRLGYTPVCRALHSL*LLRLLTQDQ*QGG
EcNanS	222	HSQLNNITDAPWFC---GDTTWYWKENFP*HAYEAIYGN*YQNNILANIIFVDF*QQ*QARG
PvSAE		-----
BfEstA		-----
pAF-AH	225	APLPEPSP-----
EcNanS	278	LTNAPDEDPDDLSTGYYSAYRSPENWTTALRSSH*FSSAARRGIISDRFVEAILQFWRER

*Residues in catalytic triad

Figure S2 Amino acid sequence alignments for a range of 9-O-SAEs. Alignments include *Phocaeicola vulgatus* PvSAE (ABR41743.1), *Bacteroides fragilis* EstA (WP_100721746.11), *Bos taurus* pAF-AH (PDBID: 3DT6) and *E. coli* NanS (PDBID: 3PT5). Residues forming the catalytic Ser-His-Asp triad are indicated with a star above the amino acid.

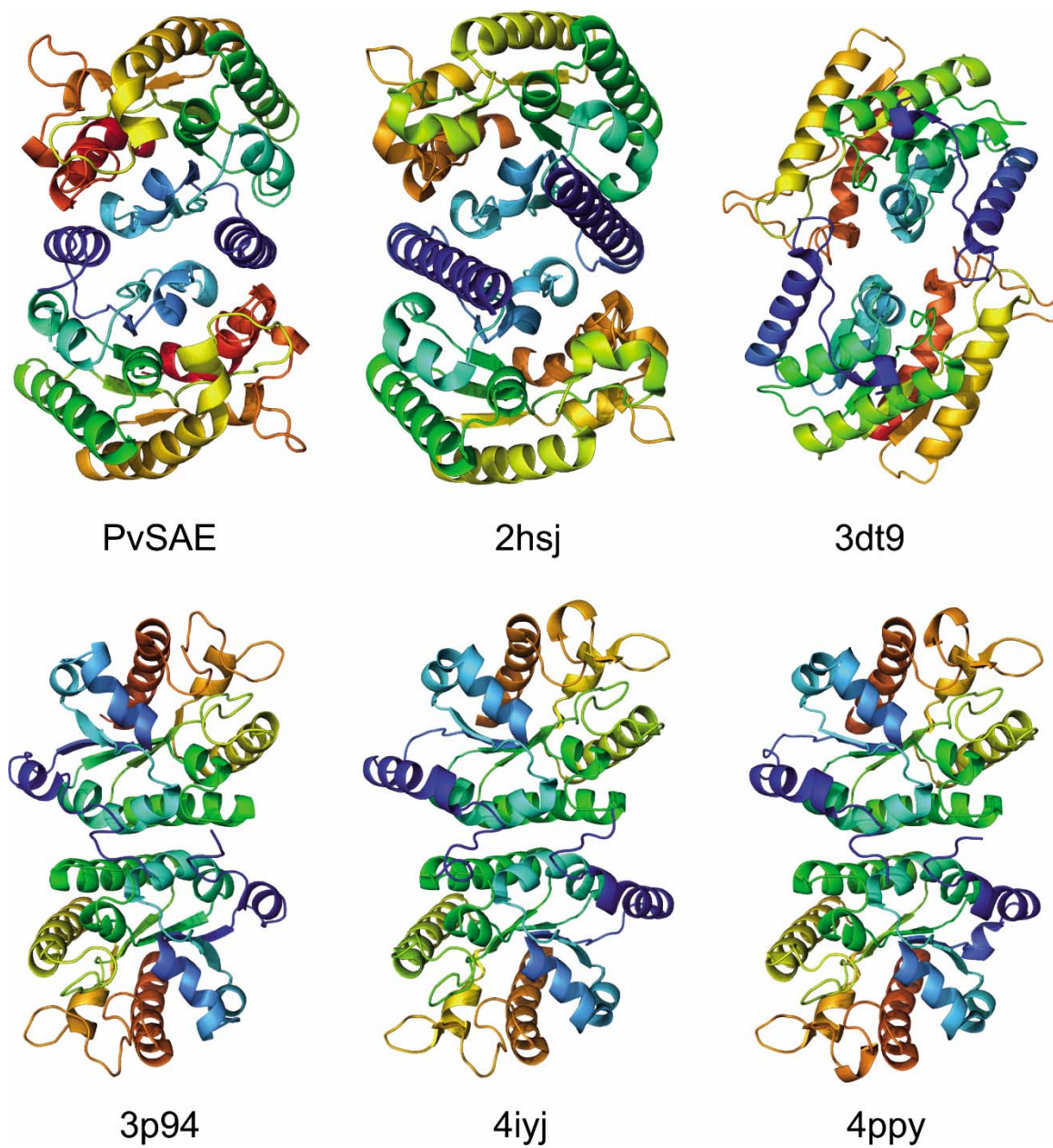


Figure S3 Dimer interfaces of PvSAE and homologs. Dimers are shown in cartoon representation and colored from the N-terminus (purple) to the C-terminus (red).

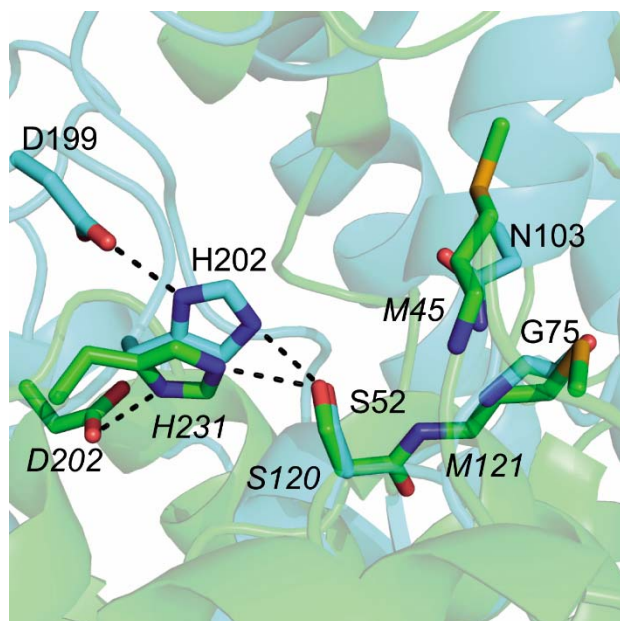


Figure S4 Active site overlay of PvSAE and *S. pneumoniae* EstA (PDB: 2uz0)(Kim *et al.*, 2008) with active site residues shown as sticks. *S. pneumoniae* EstA residues are labelled in italics and carbons are colored in green, while PvSAE carbons are cyan. Hydrogen bonds between the catalytic triad are shown as black dashed lines.

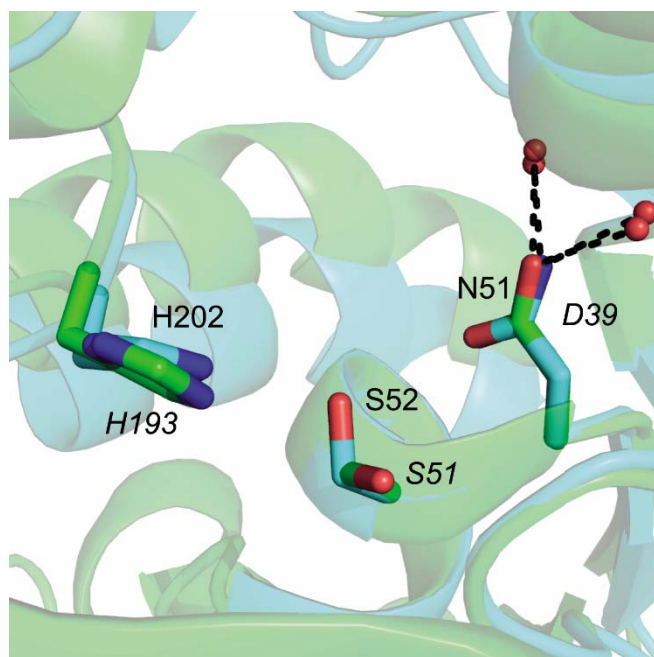


Figure S5 Active site overlay of PvSAE and *S. pneumoniae* putative platelet activating factor (PDB-ID: 2hsj) with active site residues shown as sticks. *S. pneumoniae* putative platelet activating factor residues are labelled in italics and carbons are colored in green, while PvSAE carbons are cyan. Hydrogen bonds between the catalytic triad are shown as black dashed lines.

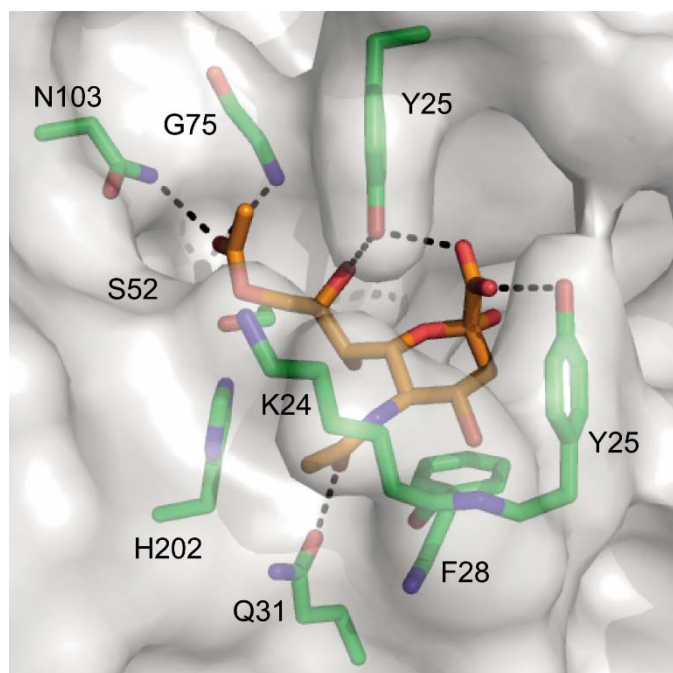


Figure S6 Docking of 9-O-acetylsialic acid into the active site of the Apo II structure. Polar interactions within 3.2 Å are shown as black dashed lines.