

**Structure and Activity Analyses of *E. coli* K-12 NagD Provide Insight
Into the Evolution of Biochemical Function in the HAD Enzyme
Superfamily^{†,‡}**

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SUPPORTING INFORMATION

1 Figure of sequence alignment of NagD homologues from various bacterial species. 2 pages total.

	1	10	20	30	40	50
E.coli_K-12
salmonella
Yersinia
Shweanella
Streptomyces
Nocardia
Leifsonia
Arthrobacter
Enterococcus faecalis
Streptococcus pneumoniae
Staphylococcus aureus
Thermotoga

	60	70	80	90	100	110
E.coli_K-12	NRFA	TAGV	VDV	DP	VS	VF
salmonella	NRFA	TAGV	VDV	DP	VS	VF
Yersinia	NRFI	TAGL	VDV	DP	VS	VF
Shweanella	NRFL	AAGL	VDV	DP	VS	VF
Streptomyces	ARLR	RMGL	EV	ES	IV	TS
Nocardia	ARLR	TTGL	LD	IP	ES	IV
Leifsonia	ARLR	ASGL	VDV	DP	VS	VF
Arthrobacter	ARLR	SSGL	EV	ES	IV	TS
Enterococcus faecalis	QRLA	NEFD	IH	VP	AS	LV
Streptococcus pneumoniae	EMLA	QNFN	ID	TE	LV	YV
Staphylococcus aureus	EKLR	EMHI	DA	KE	EV	TS
Thermotoga	RKLR	NXGV	VD	DP	VS	VF

	120	130	140	150	160	170	180
E.coli_K-12	CE	TR	SY	NW	DM	MH	KA
salmonella	CE	TR	SY	NW	DM	MH	KA
Yersinia	CE	TR	SY	NW	DM	MH	KA
Shweanella	CE	TR	SY	NW	DM	MH	KA
Streptomyces	CE	TR	TY	SE	AM	TK	AV
Nocardia	CE	TR	TY	SE	AM	TK	AV
Leifsonia	CE	TR	SY	NW	DM	MH	KA
Arthrobacter	CE	TR	TY	SE	AM	TK	AV
Enterococcus faecalis	GLD	TE	LS	YE	KV	VL	TL
Streptococcus pneumoniae	GLD	WQ	VE	YE	KF	FAT	TL
Staphylococcus aureus	GLD	EQ	VT	YE	KL	AI	TL
Thermotoga	CP	DK	TL	YE	RL	KK	AC

	190	200	210	220	230	240	250
E.coli_K-12	RA	AL	NK	MQ	AH	SE	ET
salmonella	RA	AL	NK	MQ	AH	SE	ET
Yersinia	RA	AL	NK	MQ	AH	SE	ET
Shweanella	RS	AL	NH	IG	HS	ET	VI
Streptomyces	RT	GL	NA	IG	HS	ET	VI
Nocardia	RS	AL	RI	CA	HS	ET	VI
Leifsonia	RS	AL	NK	MQ	AH	SE	ET
Arthrobacter	RS	AM	QI	DA	HS	ET	VI
Enterococcus faecalis	BR	AI	HL	GL	VE	KE	QV
Streptococcus pneumoniae	DK	AV	HL	GL	VE	KE	QV
Staphylococcus aureus	VK	AL	EL	GL	VE	KE	QV
Thermotoga	DV	IS	KE	GV	PK	ER	XV

E.coli_K-12
salmonella
Yersinia
Shweanella
Streptomyces
Nocardia	NPPG
Leifsonia	VESEF
Arthrobacter
Enterococcus faecalis
Streptococcus pneumoniae
Staphylococcus aureus	K.....
Thermotoga

Figure S1. The sequence alignment of NagD homologues from various bacterial species. In red-highlight and boxed in blue are shown the stringently conserved residues. In red text and boxed in blue are conserved residues. Accession codes for sequences or PDB: *E. coli* K-12: P15302; *Salmonella enterica*: NC_004631.1; *Yersinia pseudotuberculosis*: NC_006155.1; *Shweanella oneidensis*: NC_004347.1; *Streptomyces*: CAB65573; *Nocardia farcinica*: YP_121565; *Leifsonia xyli*: NC_006087.1; *Arthrobacter*: AAHG1000001.1; *Enterococcus faecalis* NP_814917; *Streptococcus mutans*: AAN59079; *Staphylococcus aureus*: YP_040313; *Thermotoga maritima*: NP_229540.