

SUPPORTING INFORMATION

for

ELUCIDATION OF A MONOVALENT CATION DEPENDENCE AND CHARACTERIZATION
OF THE DIVALENT CATION BINDING SITE OF THE FOSFOMYCIN RESISTANCE
PROTEIN (FosA)

Two figures (4 pages)

FIGURE 1 (Supporting Information): Multiple sequence alignment of FosA (Fos_Tn2921) and other related Fos proteins, glyoxalase I (LguL), and methylmalonyl CoA and related epimerases (Epim). The residues in bold are those aligning with the metal ligands observed in the crystal structure of human glyoxalase I.

Plurality: 2.00 Threshold: 1.00 AveWeight 1.00 AveMatch 0.54 AvMismatch - 0.40

PRETTY of: pileup_348.msf{*} December 9, 1997 09:16 ..

	1					50
FosB_Staep					MIkgin H itY	sVsniAKSIE
FofB_Stasp					MIkgin H itY	sVsniAKSIE
Fos_Tn2921					MlqsLn H ltL	aVsDLqKSVt
LguL_Neiss					..MRL L HTML	RVGnLEKSId
LguL_Syn3					..MfLL L HTMi	RVGDLDKSlq
LguL_Ecoli					..MRL L HTML	RVGDLqrSID
LguL_Salty					..MRL L HTML	RVGDLqrSia
LguL_Haein					..Mqil L HTML	RVGDLDrSiK
LguL_Vibpa					i L HTML	RVGDLDKSiK
LguL_Bjuncea	..MASEa K ES	Pa..nnpgLs	t.vrDe..AT	kgyiM q qTMF	RVkDpkasId	
LguL_Lyces	..MASEs K DS	PS..nnpgLh	a.TpDe..AT	kgyfL q qTMF	RIkDpkvSIE	
LguL_Human	..MAep q ppS	ggLtdeaaaLs	c.csDadpsT	kdfL L q q TML	RVkDpkKSId	
LguL_Psepu		mSLndLnTLp	gvTaqadpAT	aqfvFn H TML	RVkDiEKsId	
Epim_Mtuber		MtTdq	Vharhmlats	LVtgLd H vgi	aVaDLdvaIE	
Epim_B1549_Mlepr		mMtTdq	InTcqlLatT	LVitid H vgi	aVaDLnaaIs	
Epim_Vparv_C-Term						
Epim_AF2218_Afulg					MIRkid H vgv	aVksLEeaVk
Epim_D2030.5_Celeg	masfrstlal	vnsakLslst	rtmashplAg	LlgkLn H vai	atpDLkKSsE	
Epim_YqjC_Bacsu				..mnRLd H igi	aVfpikdars	
Consensus	-----	-----	-----	-----	-----	-----
	51					100
FosB_Staep	FYrDILGadi	LvegE.....				TSA
FofB_Stasp	FYrDILGadi	LvesE.....				TSA
Fos_Tn2921	FWhElLGLtL	harwn.....				TgA
LguL_Neiss	FYqnVLGMKL	LRrkDyPEgr	FtLAFvGYGD	EtD.....		St
LguL_Syn3	FYcDILGMnL	LRkkDyPsge	FtLAFvGYGk	EsE.....		na
LguL_Ecoli	FYTkVLGMKL	LRtsEnPEyK	YSLAFvGYGp	EtE.....		ea
LguL_Salty	FYTnVLGMKL	LRtsEnPEyK	YSLAFvGYGp	EtE.....		ea
LguL_Haein	FYqDVLGMrL	LRtsEnPEyK	YtLAFvGYed	ges.....		aa
LguL_Vibpa	FYTEVMGMqL	LRtnEnkEye	YtLAFvGYGD	Esq.....		ga
LguL_Bjuncea	FYsrVLGMSL	LkrlDfsEmK	FSLyFLGYeD	tstaPtDPtE	RTvWTFgrpA	
LguL_Lyces	FYskVLGMSL	LkrlDfPEmK	FSLyFMGYeD	tasaPsDPvE	RTAWTFSqks	
LguL_Human	FYTrVLGMtL	iqkcDfPimK	FSLyFLaYeD	knDiPKEkDE	kiAWaLSrkA	
LguL_Psepu	FYTrVLGFKL	vdkrDfvEaK	FSLyFLalvD	patiPaDdDa	RhqWmkSipg	
Epim_Mtuber	WYhDhLGMiL	vheevndDqg	ireALLavpg	...s.....		aa
Epim_B1549_Mlepr	WYhDhLGMiL	vheevndDqg	ireAMLsahg	apiG.....		tt
Epim_Vparv_C-Term						
Epim_AF2218_Afulg	tYea.LGFgv	eeieEvaEqK	vrivAMLpa..	...G.....		es
Epim_D2030.5_Celeg	FYkg.LGaKv	seavppqPEhg	vyytvFvel..	...p.....		ns
Epim_YqjC_Bacsu	FYenVLGLaF	LhgetveEqK	vnnvAFFqa..	...G.....		Sv
Consensus	-----	-----	-----	-----	-----	-----

	101		150
FosB_Staep	yfnLggiWla lnEekn...i	prseikysYt	HIAftTISDnD fEDwYiWLkE
FofB_Stasp	yfnLggiWla lnEekn...i	prseikysYt	HIAftTISDnD fEDwYnWLkE
Fos_Tn2921	yltcgdlWvc lsydearqYv	ppqesd..Yt	HyAftVAEED fEplsqRLeq
LguL_Neiss	VIELTHNWdT Er.....YD	LGN....aYG	HIAVeV..DD ayEACERvkr
LguL_Syn3	VIELTHNWGT Dk.....YD	LGN....GFG	HIAIgv..ED IystCDkirD
LguL_Ecoli	VIELTyNWGv Dk.....YE	LGt....aYG	HIAIsV..Dn aaEACEkirq
LguL_Salty	VIELTyNWGv Es.....YD	MGN....aYG	HIGIsV..Dn aaEACERirq
LguL_Haein	eIELTyNWGv Dk.....YE	hGt....aYG	HIAIgV..DD IyatCEavra
LguL_Vibpa	VIELTyNWGk tE.....YD	LGt....aFG	HIAIgV..DD IyatCDaika
LguL_Bjuncea	tIELTHNWGT EsDpefkgyh	nGNsEPRGFG	HIGvTV..DD VhkACERFeq
LguL_Lyces	tIELTHNWGT EsDpnftgyh	nGNsEPRGFG	HIGvTV..DD VykACERFes
LguL_Human	tIELTHNWGT EDDat.qsYh	nGNsDPRGFG	HIGIaV..pD VysACKRFeE
LguL_Psepu	VIELTHNhGT ErDadfaYh	hGNtDPRGFG	HICVsV..pD VvaACERFea
Epim_Mtuber	qIqLma..pl DESsvIAKFl	dkrG..pGiq	qIAcrV..sD lDamCrRLrs
Epim_B1549_Mlepr	qIqLma..pi nEsSPIAKFl	dkhG..pGiq	qIAcrV..sD lDrltkRLra
Epim_Vparv_C-Term	..EFle..tT tpDgPIgKFi	ekNGgrdGiq	HVAIrV..Dn IEnAiadLma
Epim_AF2218_Afulg	rVELle..aT sEDSaIAKFi	ssrG..eGih	HIAVnV..En IEEAlnkakeE
Epim_D2030.5_Celeg	kIELLH..pf gEkSPIqaFl	nkNkD.gGmh	HICIEV..rD IhEAvsavkt
Epim_YqjC_Bacsu	klgLie..pl taDSPVhlFl	ekkG..qGLh	HIAflc..nc lsEqlqaLsD
Consensus	-----	-----	-----

	151		200
FosB_Staep	neVNilegrd rdirdkKsIy	Ft...DlDGH	KIELhtgsle dRlsyykEAK
FofB_Stasp	neVNilegrd rdirdkKsIy	Ft...DlDGH	KIELhtgsle dRlsyykEAK
Fos_Tn2921	aGVti....wk qnKseGasfy	Fl...DPDGH	KIELhvgsla aRlaacrE.K
LguL_Neiss	qGgNvVREAG PmKhGttVIA	FV...eDPDGY	KIEFIqkKSg ddsavayqtA.
LguL_Syn3	kGgkvVREpG PmKhGttVIA	FV...eDPDGY	KIELIqtsSk kd.....
LguL_Ecoli	nGgNvtREAG PVKGGttVIA	FV...eDPDGY	KIELIEeKdA gRgLGn....
LguL_Salty	nGgNvtREAG PVKGGstIIA	FV...eDPDGY	KIELIEaKdA gRgLGn....
LguL_Haein	sGgNvtREAG PVKGGstVIA	FV...eDPDGY	KIEFIEnKSt ksgLGn....
LguL_Vibpa	aGgNvtREAG PVKGGtthIA	FV...KDPDGY	mIELIqnKqA sagLeg....
LguL_Bjuncea	lGVefVkk.. PhdGkmKnIA	FI...KDPDGY	wIELfDlKti gttaGnaa..
LguL_Lyces	lGVefVkk.. PldGkmKgIA	FI...KDPDGY	wIELfDtKii kdaaGsas..
LguL_Human	lGVkfVkk.. PddGkmKgIA	FI...qDPDGY	wIELInPnkm atLM.....
LguL_Psepu	lqVpfqkr.. lsdGrmnhIA	FI...KDPDGY	wVEvIqPtpl
Epim_Mtuber	qGVrlVyEta rrgtansrIn	FIHPKDagGv	lIELVEPaps
Epim_B1549_Mlepr	qGVrlVyDtp rrgtsnarIn	FIHPKDagGv	lIELVEPaS.
Epim_Vparv_C-Term	kGVrmIdEkp rygaGGssIA	FlHPKatgGv	lIELcqrnk.
Epim_AF2218_Afulg	aGlrIdEkp rVgaGGKkVA	FVHPKsthGv	lIEFVEg... ..
Epim_D2030.5_Celeg	kGIrtlgEkp kIgahGKeVm	FlHPKDcgGv	lIELeqe... ..
Epim_YqjC_Bacsu	qhVqlIdrfp rgganGKkIA	FlsPrEtnGv	lVELcEPKgd qhnehe....
Consensus	-----	F-----G-	---E-----

	201	212
FosB_Staep	PHMNFYI... ..	
FofB_Stasp	PHMNFYI... ..	
Fos_Tn2921	Pyagmvftsd ea	
LguL_Neiss		
LguL_Syn3		
LguL_Ecoli		
LguL_Salty		
LguL_Haein		

LguL_Vibpa	
LguL_Bjuncea	
LguL_Lyces	
LguL_Human	
LguL_Psepu	
Epim_Mtuber	
Epim_B1549_Mlepr	
Epim_Vparv_C-Term	
Epim_AF2218_Afulg	
Epim_D2030.5_Celeg	
Epim_YqjC_Bacsu	
Consensus	-----

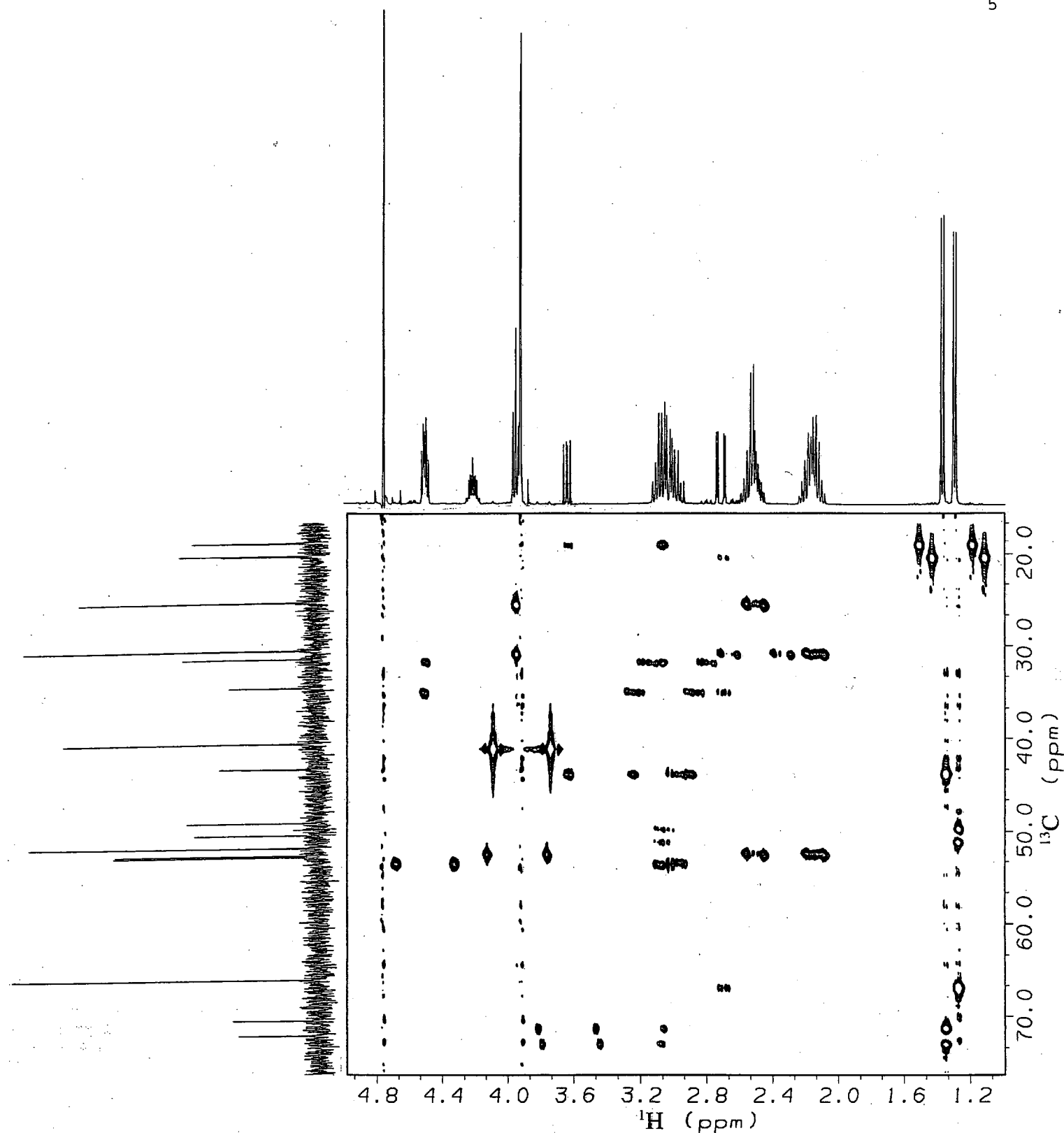


FIGURE 2 (Supporting Information): Portion of the HMBC NMR spectrum of the product mixture from the spontaneous reaction of glutathione with fosfomycin. A complete list of assignments appears in the Experimental Section.