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In silico characterization and molecular modeling of GntR family regulators in *Xanthomonas axonopodis* pv. *citri*: Implications for primary metabolism or virulence

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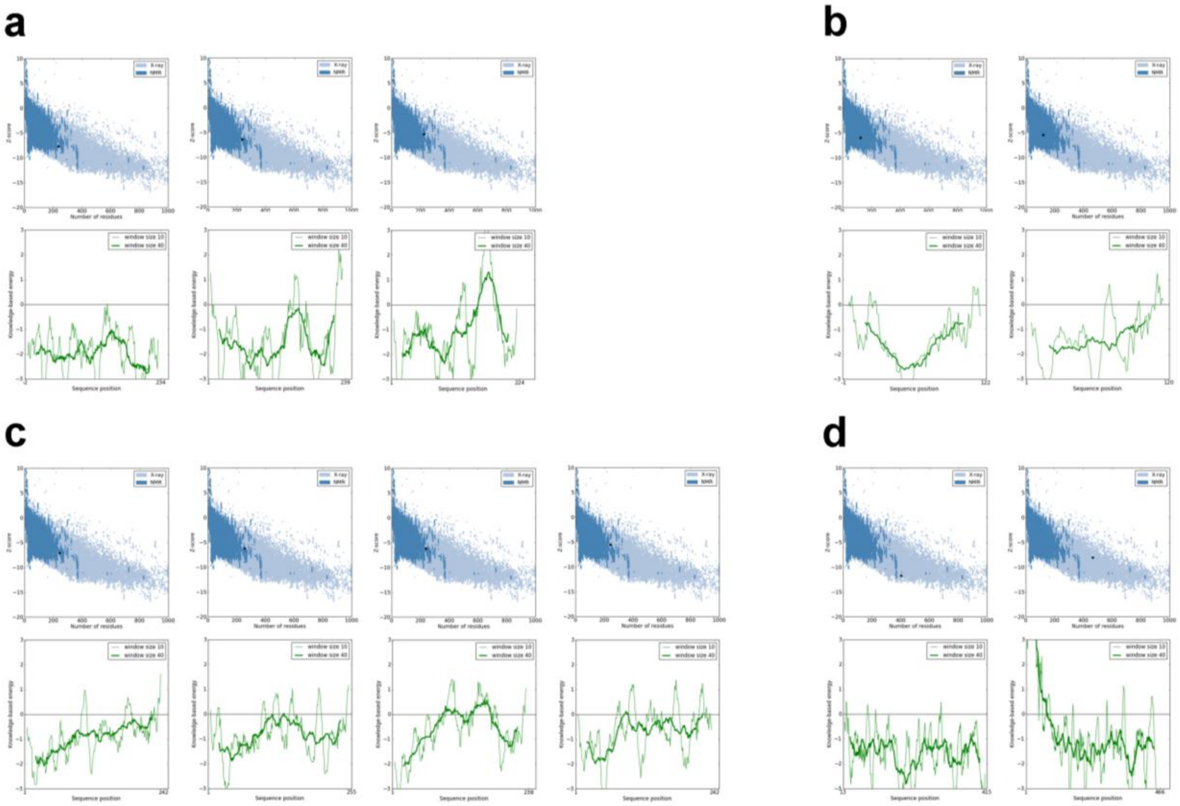
Supplementary Table S1. Details of GntR regulators used as representatives from all subfamilies.

Subfamily	Protein ID	Organism	Length (amino acids)	Swiss-Prot ID
AraR	AraR	*Bacillus stearothermophilus*	364	Q9S470
	P96711	*Bacillus subtilis*	362	P96711
	Q9KBQ0	*Bacillus halodurans*	375	Q9KBQ0
FadR	EmoR	EDTA-degrading bacterium BNC1	207	Q9F9T1
	FadR	*Escherichia coli*	238	P0A8V6
	GlcC	*Escherichia coli*	254	P0ACL5
	LldR	*Escherichia coli*	258	P33233
	MatR	*Rhizobium leguminosarum*	222	Q9JP74
	MdcY	*Acinetobacter calcoaceticus*	224	Q9F0Q8
	NtaR	*Chelatobacter heintzii*	210	P54988
	PdhR	*Escherichia coli*	254	P0ACM1
	VanR	*Acinetobacter* sp. ADP1	251	O24839
HutC	DasR	*Streptomyces coelicolor*	254	Q9K492
	FarR	*Escherichia coli*	240	P13669
	HutC	*Pseudomonas putida*	248	P22773
	PhnF	*Escherichia coli*	241	P16684
	PhnR	*Salmonella typhimurium*	239	P96061
	Q82IW0	*Streptomyces avermitilis*	254	Q82IW0
	Q8VV01	*Streptomyces griseus*	253	Q8VV01
	TreR	*Bacillus subtilis*	238	P39796
	YvoA	*Bacillus subtilis*	243	O34817
MocR	MocR	*Rhizobium meliloti*	493	P49309
	YcnF	*Bacillus subtilis*	479	P94426
	YcxD	*Bacillus subtilis*	444	Q08792
	YhdI	*Bacillus subtilis*	469	O07578
	YjiR	*Escherichia coli*	470	P39389
	YrdX	*Rhodobacter sphaeroides*	456	Q01856
PlmA	All1076	*Anabaena* sp. strain PCC 7120	328	Q8YXY0
	Sll1961	*Synechocystis* sp. strain PCC 6803	388	P73804
	Tll2117	*Synechococcus elongatus*	367	Q8DH43

YtrA	BH0651	*Bacillus halodurans*	123	Q9KF35
	BH2647	*Bacillus halodurans*	123	Q9K9J9
	SAV1934	*Staphylococcus aureus*	126	Q99SV4
	YhcF	*Bacillus subtilis*	121	P54590
	YtrA	*Bacillus subtilis*	130	O34712



Supplementary Fig S1. ProSA-web results for template protein and modeled *Xac* GntR-like regulators. Z-plot graphs **(*upper panel*)** show spots of Z score's values of proteins determined by NMR (represented in dark blue colour) and by X ray (represented in light blue colour). The black dots represent Z-Scores of our models and their coresponding templates, and e-plot graphs **(*lower panel*)** show local model quality by plotting energies as a function of amino acid sequence position *i*. In general, positive values correspond to problematic or erroneous parts of the input structure. The plots are smoothed by calculating the average energy over each 40-residue fragment s(*i*,*i*+39), which is then assigned to the 'central' residue of the fragment at position *i*+19 (thick line). A second line with a smaller window size of 10 residues is shown in the background of the plot (thin line). **(a)** Left, 3C7J (A chain); middle, XAC0568; right, XAC0877. **(b)** Left, 3BY6 (E chain); right, XAC1548. **(c)** From left to right. 2WV0 (D chain), XAC0711, XAC1640 and XAC3532. **(d)** Left, 1WST (A chain); right, XAC0737.