Table S2. *In silico* analysis of adenylation domains in xantholysin synthetases. Predicted substrate specificity of the A domains in the xantholysin NRPSs.

Protein	Domain	NRPSpredictor2 Signature	Motif	AA (score)	Phylotree[a]
XtlA	A1	LWHAFDAMAWEPFLLVG GDINNYGPTEATVVASA	DAWFLGNVVK	Leu (100%)	Leu
	A2	LWGAFDGSVWEWKFFCG GGHNVYGPTEATVDSTA	DGWKFGVVDK	Asp (70%)	Glu
XtlB	A3	LWATFDASVWEWQFVCG GGHNVYGPTETTVDCTV	DAWQVGVVDK	Gln (70%)	Gln
	A4	LNNSFDASTLEAWLMVG GDLNGYGPTEATTFSTT	DALWMGGTFK	Val (80%)	Val
	A5	LWHAFDAMAWEPFLLVG GDVNNYGPTETTVVATS	DAWFLGNVVK	Leu (100%)	Leu/Ile
	A6	LWSTFDASVWEWQFVCG GGHNVYGPTETTVDCSV	DAWQVGVVDK	Gln (70%)	Gln
	A7	RWMTFDVSVWEWHFLCS GEHNLYGPTEAAVDVSA	DVWHLSLVDK	Ser (80%)	Ser
	A8	LNNSFDASTLEAWLMVG GDLNGYGPTEATTFSTT	DALWMGGTFK	Val (80%)	Val
	A9	LWHAFDAMAWEPFLLVG GDVNNYGPTETTVVATS	DAWFLGNVVK	Leu (100%)	Leu/Ile
	A10	LWSTFDASVWEWQFVCG GGHNVYGPTETTVDCSV	DAWQVGVVDK	Gln (70%)	Gln
XtlC	A11	LWHAFDAMAWEPFLLIG GDVNNYGPTETTVVASS	DAWFLGNVVK	Leu (100%)	Leu
	A12	LWHAFDAMAWEPFLLIG GDVNNYGPTEATVVATS	DAWFLGNVVK	Leu (100%)	Leu
	A13	LWSTFDASVWEWQFVCG GGHNVYGPTEATVDCSV	DAWQVGVVDK	Gln (70%)	Gln
	A14	LNNSFDAATLDGFVLCG GEVHCYGPTETTTFATA	DALFLGCTFK	Leu (70%)	Ile/Val/Leu

[a] Deduced from A domain clustering in Fig. 3