Supplemental data for:

Investigating inducible short-chain alcohol dehydrogenases/reductases clarifies rice oryzalexin biosynthesis

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Figure S1. Alignment of SDRs investigated in this report. The TGxxxGxG coenzyme binding and catalytic YxxxK motifs are underlined, while the Asp residue indicating the preference for NAD⁺ over NADP⁺ is indicated by an asterisk. Note that OsSDR110C-MI4 appears to be truncated at the N-terminus relative to the other MI clade members, and may represent a pseudo-gene.

	20		40		60		
OCMAS/SDR110C-MS1	MAAC		C C L		CKNANTCCA	SCUCACTAR	26
OSMAS/SDR110C-MS1	MAAG				CKWAWLTCCA	SCICACTARL	25
OrSDR110C-MS2	MAC		S S NC		CKWALLTCCA	SCICECTARI	33
OcsDR110C-M33			S DACENSCES		CKWANITCCA	SCICKATAKE	60
OSSERTIOC-MIS		EINNALGAAI	SFAUENSUES	I A SIN SAUREA	CKWALLTCCA	SCICKNTAKE	20
Os5DR110C-MI4		DCDDTDAASS			CKWANITCCA	SCICRATARE	50
OSSERTIOC-MIZ		NUNNIPANJJ	33WINEA		UNVAVII UUA	JUIUNAIAEE	1 30
		1		100		120	1
OsMAS/SDR110C-MS1	FVKHGARVVV	ADIQDELGAS	LVAELGPDAS	S YVHC DVT NE	GDVAAAVDHA	VARFGKLDVN	96
OsSDR110C-MS2	FVKHGARVVV	ADIQDELGAS	LVAELGPDAS	S YVHC DVT NE	GDVAAAVDHA	VATEGKLDVM	95
OsSDR110C-MS3	FVK HGAQVVV	ADIQDEAGAR	LCAELGSATA	S YVR C DVT S E	DDVAAAVDHA	VARYGKLDVN	97
OsSDR110C-MI3	FIENGAKVIM	A DV Q D D L G H S	TAAELGPDA-	SYTRCDVTDE	AQVAAAVDLA	VKRHGHLDIL	119
OsSDR110C-MI4	FIKNGAKVII	ADVQDELGHS	AAA <mark>K L</mark> G P D A –	SYTHCDVTDE	AQVEAAVDLA	VRLHGHLDIL	89
OsSDR110C-MI2	FVRNGAKVIL	ADVQDDLGHA	VAAELGADAA	SYARCDVTDE	AQVAAAVDLA	VARHGRLDVV	116
		* 140		160		180	1
OCMAS/SDB110C MS1		DCEDMSECT					1.54
OSMAS/SDR110C-MS1		PCERITEST					154
OrsDR110C-MS2							155
OSSDR110C-M33						CH LLCTASE	170
OSSDR110C-MIS		PODDMASVDL					1/0
OcsDR110C-MI2							140
OSSDR110C-MIZ							1/3
		1		220		240	1
OsMAS/SDR110C-MS1	SSSVSGAASH	AYTTSKHALV	GETENAAGEL	GRHGIRVNCV	S P A G V A T P L A	RAAMGMD	211
OsSDR110C-MS2	S S S V S G T A S H	AYTTSKRALV	GETENAAGEL	GRHGIRVNCV	SPAAVATPLA	RAAMGMD	210
OsSDR110C-MS3	A <mark>S</mark> A V A G T A S H	AYTCAKRALV	GLTENAAAEL	GRHGIRVNCV	S P A A A A T P L A	TGYVGL E	213
OsSDR110C-MI3	TGVMPMPNIA	LYAVSKATTI	A I V R AAA E P L	SRHGLRVNAI	S P H G T R T P M A	MHVLSQMYPC	238
OsSDR110C-MI4	AG <mark>VMPIPNI</mark> A	MYSVSKATTI	A I V R AAA E P L	SRHGLRVNAL	S P T G T R T P M M	MHIISQMTPC	208
OsSDR110C-MI2	AGVIGGVAVP	HY <mark>SVSK</mark> AAVL	GLVRAVAGEM	A <mark>r s</mark> gvrvna i	S P N Y I WT P MA	AVAFARWYPS	235
		260		280		300	1
OcMAS/SDR110C_MS1					VVSCONERVE		268
OsDR110C-MS2		EKSANLKCVC			VVS CONLEVE	CCVSVVN-SS	268
OsSDR110C-MS2		FAVANLKCV-	RERVEDIAAA		VVSCHNELID	CCCSIVN-PS	269
OsSDR110C-MI3					YVNCHNLVVD	COLLENKOS	296
OSDR110C-MI4					YVNCHNLVVD	CCETTHKCD	266
OSDR110C-MI2	RSADDHRRIV			AVELASDEAK	YVNCHNLVVD	CCYTYCKYPN	295
035571100-1012							233
OSMAS/SDR110C-MS1	EGEERD- 274						
OsSDR110C-MS2	FGFFRD- 274						
OsSDR110C-MS3	EGIEKD* 276						
OsSDR110C-MI3	IRLN 300						

OsSDR110C-MI4 NRM---N 270 OsSDR110C-MI2 MPVPDGH 302

OsMAS/SDR110C-MS1 Ρ S OsSDR110C-MS2 Total Ion Counts Total Ion Counts S Р l 17.0 Retention Time (min.) 16.5 17.5 17.5 16.5 16.0 17.0 18.0 16.0 18.0 Retention Time (min.) OsSDR110C-MI3 OsSDR110C-MS3 Р Total Ion Counts Total Ion Counts Ρ 16.5 17.5 1 17.5 17.0 Retention Time (min.) 16.0 16.0 18.0 16.5 17.0 18.0 Retention Time (min.) 91 P (3-keto-*syn*-pimaradiene) S (3β-hydroxy-syn-pimaradiene) 255 286 105 119 lon Counts lon Counts 257 229 227 288 200 *m/z* 200 100 150 250 150 250 300 300 100 m/z (minin (minin H H HO 0

Figure S2. SDR activity with the simplified substrate analog 3β -hydroxy-*syn*-pimaradiene. GC-MS chromatograms for each active SDR, mass spectra for the substrate and product, and catalyzed oxidation reaction.

Figure S3. SDR activity with the simplified substrate analog 2α -hydroxy-*ent*-cassadiene. GC-MS chromatograms for each active SDR, mass spectra for the substrate and product, and catalyzed oxidation reaction.



Figure S4. SDR activity with the simplified substrate analog 3α -hydroxy-*ent*-cassadiene. GC-MS chromatograms for each active SDR, mass spectra for the substrate and product, and catalyzed oxidation reaction.



Figure S5. SDR activity with the simplified substrate analog 3α -hydroxy-*ent*-sandaracopimaradiene. GC-MS chromatograms for each active SDR, mass spectra for the substrate and product, and catalyzed oxidation reaction.



Figure S6. SDR activity with the simplified substrate analog 7β -hydroxy-*ent*-sandaracopimaradiene. GC-MS chromatograms for the active SDR110C-MS3, mass spectra for the substrate and product, and catalyzed oxidation reaction.



Sequence of synthetic OsSDR110C-MS2