

Supplementary Materials

Identification and *in silico* molecular modelling study of newly isolated *Bacillus subtilis* SI-18 strain against S9 protein of *Rhizoctonia solani*

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Table S1. The list of species and GenBank accession numbers of DNA sequences for constructing the phylogenetic tree

Species	Strain	Host	Location	Accession no.	
				16S rRNA	<i>gyrB</i>
<i>Bacillus subtilis</i>	SI-18	Wheat root	China	MT598066	MW008865
	BCRC 14716	Rhizosphere flax	Taiwan	EF423595.1	DQ309314.1
	BCRC 17435	Rhizosphere flax	Taiwan	EF423598.1	DQ309317.1
	GA2(1)	Soyabean oil	Taiwan	MH700783.1	MG025594.1
<i>Bacillus amyloliquefaciens</i>	DY1b	Unknown	China	KY290588.1	KY315726.1
<i>Bacillus licheniformis</i>	BCRC 15413	Rhizosphere flax	Taiwan	DQ993676.1	DQ309325.1

<i>Bacillus mojavenensis</i>	UEBFK	Garlic	Tunisia	KC297104.1	JQ916083.1
<i>Bacillus pumilus</i>	SB6	Sugar beet	Iran	KR092173.1	KR092180.1
<i>Bacillus safensis</i>	FO-036b	Biofilms	USA	AF234854.2	AY167868.1
<i>Bacillus altitudinis</i>	PG-5	Promagenate seed	China	MN435571.1	MN893287.1
<i>Bacillus aerophilus</i>	MCCC 1A08371	Unknown	China	JX680141.1	JX680218.1
<i>Bacillus thuringiensis</i>	KS	Unknown	Tunisia	KC737848.1	KC737849.1
<i>Bacillus megaterium</i>	IARI-AR44	Soil	India	KJ433619.1	KJ474961.1
<i>Vibrio rotiferianus</i>	HM-10	Hippocampus	China	KX962166.1	KX962168.1

Table S2 List of antimicrobial compounds from *Bacillus subtilis*

Serial Number	Compound Name	References	Serial Number	Compound Name	References
1	Entianin	Fuchs <i>et al.</i> , 2011	68	2,4-Heptadienal, (E,E)-, 2-Decenal, (E)-, 2-Heptenal, (Z)-, 2-Nonenal, (E)-, 2-Octenal, (E)-, 2-Undecenal, 2,4 Decadienal, Octanal	Liu <i>et al.</i> , 2008
2	Ericin A	Stein <i>et al.</i> , 2002	69	Decanal	Yuan <i>et al.</i> , 2012b
3	Ericin S	Agrios, 1988	70	Nonanal	Wang <i>et al.</i> , 2013
4	Subtilin	Heinzmann <i>et al.</i> , 2006	71	Eicosane, 10-methyl-	Raza <i>et al.</i> , 2016
5	Mersacidin	Brötz <i>et al.</i> , 1995	72	Heneicosane	Chen <i>et al.</i> , 2008
6	Sublancin 168	Paik <i>et al.</i> , 1998	73	Heptadecane	Zheng <i>et al.</i> , 2013
7	Lichenicidin	Begley <i>et al.</i> , 2009	74	Heptadecane, 2,6,10,15-tetramethyl-	Raza <i>et al.</i> , 2016
8	Subtilosin A	Shelburne <i>et al.</i> , 2007	75	Heptane, 2-methyl-7-oxabicyclo[2.2.1]	Chen <i>et al.</i> , 2008
9	Lichenin	Pattnaik <i>et al.</i> , 2001	76	Heptane, 2-methyl-7-oxabicyclo[2.2.1]	Liu <i>et al.</i> , 2008
10	Bac 14B	Hammami <i>et al.</i> , 2012	77	Hexadecane, 2,6,11,15-tetramethyl-	Wang <i>et al.</i> , 2013
11	Baciamin	Wong <i>et al.</i> , 2008	78	Nonadecane, 9-methyl-	Chen <i>et al.</i> , 2008

12	Amylocyclicin	Scholz <i>et al.</i> , 2014	79	Nonadecane,10-methyl-	Chen <i>et al.</i> , 2008
13	Sonorensin	Chopra <i>et al.</i> , 2014	80	Pentadecane	Chen <i>et al.</i> , 2008
14	Plantazolicin	Scholz <i>et al.</i> , 2011	81	Pentadecane, 8-hexyl-	Wang <i>et al.</i> , 2013
15	CAMT2	An <i>et al.</i> 2015	82	Tetradecane	Chen <i>et al.</i> , 2008
16	Bacisubin	Liu <i>et al.</i> , 2007	83	Tetradecane, 2,6,10- trimethyl-	Wang <i>et al.</i> , 2013
17	Amylolysin	Arguelles Arias <i>et al.</i> , 2013	84	Undecane,1,2-methyl	Chen <i>et al.</i> , 2008
18	Chitinase	Podile and Prakash, 1996	85	1H-indene, 1-methylene-	Wang <i>et al.</i> , 2013
19	AHL-lactonases	Pan <i>et al.</i> , 2008	86	1,3-butadiene	Liu <i>et al.</i> , 2008
20	Agrastatin A	Lee and Kim, 2015	87	1-decene, 8-methyl-	Tahir <i>et al.</i> , 2017
21	Fengycin	Zhao <i>et al.</i> , 2014	88	1,3- pentadiene	Liu <i>et al.</i> , 2008
22	Fengycin A	alfanova <i>et al.</i> , 2012	89	β -Benzeneethanamine	Gotor-Vila <i>et al.</i> , 2017
23	Fengycin B	Li <i>et al.</i> , 2012	90	1,2-Benzisothiazol-3(2H)- one	Zheng <i>et al.</i> , 2013
24	Fengycin C, D, S	Li <i>et al.</i> , 2012	91	2,4-bis(2-Methylpropyl)- phenol	Tahir <i>et al.</i> , 2017
25	Plipastatin	Gao L. <i>et al.</i> , 2017	92	2-Phenylethanol	Chen <i>et al.</i> , 2008
26	Bacillomycin	Romero <i>et al.</i> , 2007	93	4-Hydroxybenzaldehyde	Raza <i>et al.</i> , 2016
27	Bacillomycin D	Tanaka <i>et al.</i> , 2014	94	4-Hydroxybenzaldehyde	Chen <i>et al.</i> , 2008
28	Bacillomycin F	Lee <i>et al.</i> , 2008	95	Benzene, 1,2,4,5-tetramethyl	Wang <i>et al.</i> , 2013
29	Bacillomycin L	Zhang <i>et al.</i> , 2013	96	Benzene, 1,2,4-trimethyl	Tahir <i>et al.</i> , 2017

30	Bacillomycin LC	Eshita <i>et al.</i> , 1995	97	Benzene, 1-methyl-4-(1-methylethyl)-	Chen <i>et al.</i> , 2008
31	Bacillomycin R	Besson <i>et al.</i> , 1976	98	Benzene, 2-propenyl	Yuan <i>et al.</i> , 2012b
32	Eumycin	Besson <i>et al.</i> , 1976	99	Benzene,1,4-dichloro	Yuan <i>et al.</i> , 2012b
33	Iturin	Cawoy <i>et al.</i> , 2014	100	Benzothiazole	Wang <i>et al.</i> , 2013
34	Iturin A	Gong <i>et al.</i> , 2015	101	Benzene,1,4-dichloro	Wang <i>et al.</i> , 2013
35	Iturin C	Dunlap <i>et al.</i> , 2011	102	Benzothiazole	Yuan <i>et al.</i> , 2012b
36	Iturin D, E	Besson and Michel, 1986	103	Butylated hydroxytoluene	Gao Z. <i>et al.</i> , 2017
37	Mycosubtilin	Fickers <i>et al.</i> , 2009	104	Ethylbenzene	Zheng <i>et al.</i> , 2013
38	Subtulene A	Thasana <i>et al.</i> , 2010	105	Ethylbenzene	Yuan <i>et al.</i> , 2012b
39	Bamylocin A	Lee <i>et al.</i> 2007	106	Phenol, 2,4-bis(1,1-dimethylethyl)	Yuan <i>et al.</i> , 2012b
40	Lichenysin	Jenny <i>et al.</i> , 1991	107	Phenol, 4,4'-(1-methylethylidene) bis-	Gao Z. <i>et al.</i> , 2017
41	Lichenysin A	Yakimov <i>et al.</i> 1995	108	Phenol, 4-chloro-3-methyl	Raza <i>et al.</i> , 2016
42	Locillomycin	Luo <i>et al.</i> , 2015	109	Phenol,2,3,6-trimethyl-	Gao Z. <i>et al.</i> , 2017
43	Pumilacidin A, B, C, D, E, F, G	Saggesse <i>et al.</i> , 2018	110	P-xylene	Yuan <i>et al.</i> , 2012b
44	Surfactin	Gao L. <i>et al.</i> , 2017	111	P-xylene	Yuan <i>et al.</i> , 2012b
45	WH1 fungin	Qi <i>et al.</i> , 2010	112	Styrene	Wang <i>et al.</i> , 2013
46	Bacilysin	Caulier <i>et al.</i> , 2018	113	Toluene	Yuan <i>et al.</i> , 2012b
47	Chlorotetain	Wang <i>et al.</i> , 2015	114	Ethyl acetate	Yuan <i>et al.</i> , 2012b

48	Bacillibactin	Yu <i>et al.</i> , 2011	115	Furan, 2-pentyl-	Chaves-Lopez <i>et al.</i> , 2015
49	Bacitracin A, F	Furuta <i>et al.</i> , 2018	116	Acetoin	Liu <i>et al.</i> , 2008
50	Mycobacillin	Majumdar and Bose, 1958	117	Acetoin	Arrebola <i>et al.</i> , 2010
51	Rhizocticin A	Kugler <i>et al.</i> , 1990	118	Butan-2-one	Gotor-Vila <i>et al.</i> , 2017
52	Butanoic acid, 3-methyl	Chaves-Lopez <i>et al.</i> , 2015	119	Butanone, 3-hydroxy-2-	Chaves-Lopez <i>et al.</i> , 2015
53	Gentisic acid	Zheng <i>et al.</i> , 2013	120	Dodecan-2-one	Chaves-Lopez <i>et al.</i> , 2015
54	n-Hexanoic acid	Raza <i>et al.</i> , 2016	121	Ethanone, 1-(4-methylphenyl)	Zheng <i>et al.</i> , 2013
55	n-Hexadecanoic acid	Zheng <i>et al.</i> , 2013	122	Pentanone, 2,2,4-trimethyl-3-	Wang <i>et al.</i> , 2013
56	Octadecanoic acid, Propanoic acid, 4-hexen-1-yl ester	Liu <i>et al.</i> , 2008	123	Propan-2-one	Yuan <i>et al.</i> , 2012b
57	Oleic acid	Liu <i>et al.</i> , 2008	124	Tridecan-2-one	Wang <i>et al.</i> , 2013
58	Propanoic acid, 2-methyl	Raza <i>et al.</i> , 2016	125	Pentanone, 2,2,4-trimethyl-3-	Wang <i>et al.</i> , 2013
59	3,4-dimethyl-5-hexen-3-ol, Heptanol	Liu <i>et al.</i> , 2008	126	1H-imidazole, 1-ethyl	Wang <i>et al.</i> , 2013
60	2-Undecanol	Chaves-Lopez <i>et al.</i> , 2015	127	Ammonium acetate	Chen <i>et al.</i> , 2008

61	1-Butanol	Liu <i>et al.</i> , 2008	128	Pyrazine, 2,5-dimethyl	Yuan <i>et al.</i> , 2012b
62	1-Butanol, 3-methyl-	Yuan <i>et al.</i> , 2012b	129	Pyrazine, 2-ethyl-3,5-dimethyl	Zheng <i>et al.</i> , 2013
63	1-Butanol	Chaves-Lopez <i>et al.</i> , 2015	130	Pyrazine, tetramethyl-	Raza <i>et al.</i> , 2016
64	1-Butanol, 3-methyl-	Liu <i>et al.</i> , 2008	131	Pyrazine,2,3,5,6-tetramethyl	Wang <i>et al.</i> , 2013
65	2,4-Heptadienal, (E,E)-, 2-Decenal, (E)-, 2-Heptenal, (Z)-, 2-Nonenal, (E)-, 2-Octenal, (E)-, 2-Undecenal, 2,4 Decadienal, Octanal	Chaves-Lopez <i>et al.</i> , 2015	132	Carbon disulphide	Liu <i>et al.</i> , 2008
66	Decanal	Chen <i>et al.</i> , 2008	133	Dimethyl trisulfide	Chaves-Lopez <i>et al.</i> , 2015
67	Nonanal	Yuan <i>et al.</i> , 2012b	134	Thiophene	Raza <i>et al.</i> , 2016

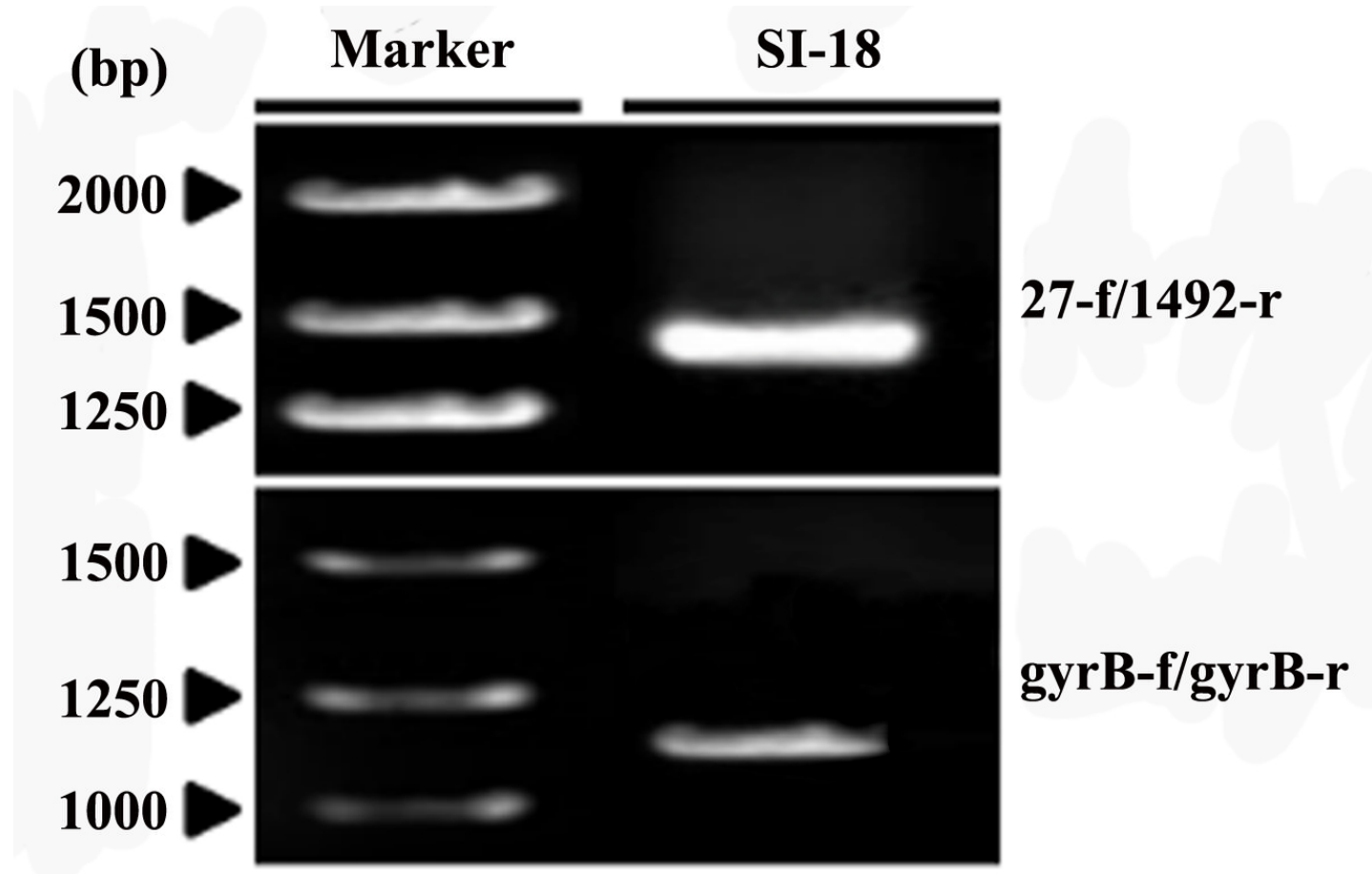


Fig. S1 PCR fragments of *B. subtilis* SI-18 strain were amplified with 27Ff/1492R and gyrB-f/gyrB-r primer pairs in -1490 bp and -1200 bp region, respectively.

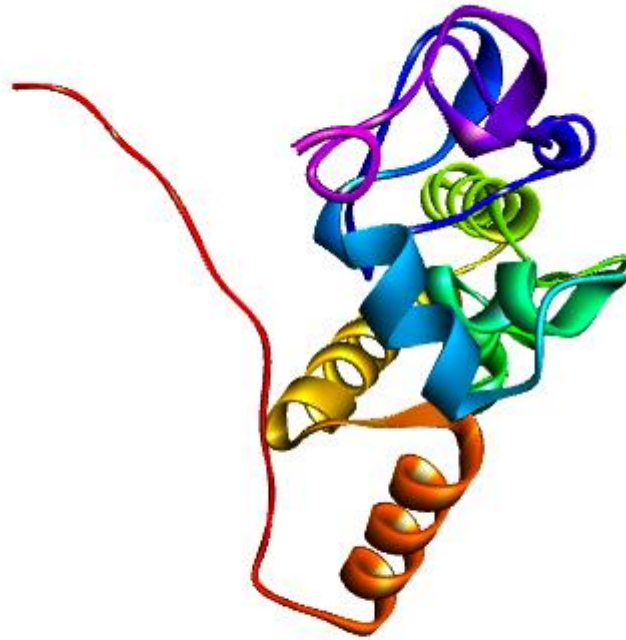


Fig. S2 Predicted protein structure obtained from SWISS-Mode.