

Virtual screening of rice phytochemical scaffolds targeting peptide deformylase of *Xanthomonas oryzae* pv. *oryzae* for the control of bacterial leaf blight

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Supplementary Data

Table S1 — List of the phytochemical extracted from different part of rice plants

Sl. No	Name of compounds	Rice Plant/Source	Nature of compound	Biological activity and function	References
1.	Sarocladiolactone A	<i>Oryzarufifipogon</i> Griff.	Helvolic acid derivatives	Antimicrobial activity	Zhang Z et al. 2021
2.	Sarocladiolactone B	<i>Oryzarufifipogon</i> Griff.	Helvolic acid derivatives	Antimicrobial activity	Zhang Z et al. 2021
3.	Helvolic acid	<i>Oryzarufifipogon</i> Griff.	Helvolic acid derivatives	Antimicrobial activity	Zhang Z et al. 2021
4.	6-deacetoxy helvolic acid	<i>Oryzarufifipogon</i> Griff.	Helvolic acid derivatives	Antimicrobial activity	Zhang Z et al. 2021
5.	Helvolinic acid	<i>Oryzarufifipogon</i> Griff.	Helvolic acid derivatives	Antimicrobial activity	Zhang Z et al. 2021
6.	1,2-dihydrohelvolic acid	<i>Oryzarufifipogon</i> Griff.	Helvolic acid derivatives	Antimicrobial activity	Zhang Z et al. 2021
7.	<i>p</i> -Hydroxybenzaldehyde	Bran	Phenolic acid	Antioxidant activity	Wang W et al 2015
8.	<i>p</i> -Hydroxybenzoic acid	Root exudate	Phenolic acid	Allelopathic effect	Seal et al 2004
9.	<i>p</i> -Hydroxy methyl benzoate glucoside	Bran	Phenolic acid	Antioxidant activity	Wang W et al 2015
10.	<i>p</i> -Hydroxy phenyl acetaldehyde	Husk and bran	Phenolic acid	-	Ding et al. 2019
11.	<i>p</i> -Hydroxy phenyl acetic acid	Husk and bran	Phenolic acid	-	Ding et al. 2019
12.	2-Hydroxy 5-[(3 <i>S</i>)-3-hydroxybutyl] phenyl β-D-glucoside (HHPG)	Bran of Purple rice	Phenolic acid	Inhibitory activity on tunicamycin-induced retinal damage	Tanaka et al 2013
13.	Caffeic acid	Endosperm/ Bran/embryo of <i>indica</i> variety	Phenolic acid	Antioxidant activity	Ti et al 2014
14.	Methyl caffeate	Bran	Phenolic acid	Antioxidant activity	Wang W et al 2015
15.	Caffeoylquinic acid methyl ester	Grains of brown rice	Phenolic acid	-	Zeg et al 2019
16.	Protocatechuic acid	Bran/embryo of <i>indica</i> variety	Phenolic acid	Antioxidant activity	Ti et al 2014
17.	Cinnamic acid	Husk and bran	Phenolic acid	-	Ding et al. 2019
18.	<i>o</i> -Coumaric acid	Bran/embryo of <i>indica</i> Root exudate	Phenolic acid	Antioxidant activity Allelopathic effect	Ti et al 2014 Seal et al 2004
19.	<i>m</i> -Coumaric acid	Grains	Phenolic acid	-	Zaupa et al 2015
20.	<i>p</i> -Coumaric acid	Grains	Phenolic acid	-	Zaupa et al 2015

21.	3- <i>O-p</i> -Coumaroyl quinic acid	Grains of brown rice Leaves	Phenolic acid	- -	Zeng et al 2019 Yang et al 2014
22.	<i>trans</i> -Ferulic acid	Bran/embryo of indica variety	Phenolic acid	Antioxidant activity	Ti et al 2014
23.	<i>trans</i> -Ferulic acid methyl ester	Bran	Phenolic acid	Antioxidant activity	Wang W et al 2015
24.	<i>cis</i> -Ferulic acid	Bran	Phenolic acid	Antioxidant activity	Wang W et al 2015
25.	<i>cis</i> -Ferulic acid methyl ester	Bran	Phenolic acid	Antioxidant activity	Wang W et al 2015
26.	1,3- <i>O</i> -Diferuloylglycerol	Leaves	Phenolic acid	-	Yang et al 2014
27.	1- <i>O</i> -Feruloyl- β -D-glucose	Leaves	Phenolic acid	-	Yang et al 2014
28.	3- <i>O</i> -Feruloylquinic acid	Leaves	Phenolic acid	-	Yang et al 2014
29.	Gallic acid	Bran/embryo of indica variety	Phenolic acid	Antioxidant activity	Ti et al 2014
30.	<i>m</i> -Salicylic acid	Grains of brown rice	Phenolic acid	-	Zeng et al 2019
31.	Salicylic acid	Rice seedlings	Phenolic acid	Disease resistance activity	Silverman et al 1995
32.	Salicylic acid 2- <i>O</i> - β -D-glucopyranoside	Leaves	Phenolic acid	-	Yang et al 2014
33.	Sinapic acid	Grains	Phenolic acid	-	Zaupa et al 2015
34.	1- <i>O</i> -Sinapoyl- β -D-glucose	Leaves	Phenolic acid	-	Yang et al 2014
35.	Syringaldehyde	Grains of brown rice	Phenolic acid	-	Zeng et al 2019
36.	Syringic acid	Bran/embryo of indica	Phenolic acid	Antioxidant activity	Ti et al 2014
37.	Vanillic aldehyde	Bran	Phenolic acid	Antioxidant activity	Wang W et al 2015
38.	Vanillic acid	Root exudate Husk and bran Grains of brown rice	Phenolic acid	Allelopathic effect - -	Seal et al 2004 Ding et al. 2019 Zeng et al 2019
39.	Apigenin 6- <i>C</i> - α -L-arabinosyl-8- <i>C</i> - β -L-arabinside	Leaves	Flavones	-	Yang et al 2016
40.	Chrysoeriol 7- <i>O</i> -rutinoside	Grains of brown rice	Flavones	-	Zeng et al 2019
41.	Chrysoeriol 6- <i>C</i> - α -L-arabinosyl-8- <i>C</i> - β -L-arabinside	Leaves	Flavones	-	Yang et al 2016
42.	5,7,4'-Trihydroxy-3',5'-dimethoxyflavone	Leaves Leaves Seedlings	Flavones	Antifungal activity Allelopathic activity Allelopathic activity	Kong et al 2004 Kong et al 2004 Kong et al 2007
43.	5,4'-Dihydroxy-3',5'-dimethoxy-7- <i>O</i> - β -glucopyranosylflavone	Seedlings	Flavones	-	Kong et al 2007
44.	7,4'-Dihydroxy-3',5'-dimethoxy-5- <i>O</i> - β -glucopyranosylflavone	Seedlings	Flavones	-	Kong et al 2007
45.	Isoscoparin 2- <i>O</i> -(6-(<i>E</i>)-feruloyl)-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
46.	Isoscoparin 2''- <i>O</i> -(6'''-(<i>E</i>)- <i>p</i> -coumaroyl)-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
47.	Isovitexin 2''- <i>O</i> -(6'''-(<i>E</i>)-feruloyl)-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
48.	Isovitexin 2''- <i>O</i> -(6'''-(<i>E</i>)- <i>p</i> -coumaroyl)-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
49.	Isoorientin 7,3'-dimethyl ether	Leaves	Flavones	-	Yang et al 2016
50.	luteolin 6- <i>C</i> -(2''- <i>O</i> - β -D-glucopyranosyl)- α -L-arabinside	Leaves	Flavones	-	Yang et al 2016

51.	Schaftoside	Leaves	Flavones	Antifeedant activity	Besson et al 1985
52.	Isoschaftoside	Leaves	Flavones	Antifeedant activity	Besson et al 1985
53.	Swertisin	Leaves	Flavones	Antifeedant activity	Yang et al 2016
54.	Tricin	Bran	Flavones	DPPH red. sca. acti.	Ajitha et al 2012
55.	Tricin 7- <i>O</i> - β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
56.	Tricin 5- <i>O</i> - β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
57.	Tricin 7- <i>O</i> -rutinoside	Leaves	Flavones	-	Yang et al 2016
58.	Tricin 7- <i>O</i> -neohesperidoside	Leaves	Flavones	-	Yang et al 2016
59.	Tricin 7- <i>O</i> -(2"- <i>O</i> - β -D-glucopyranosyl)- β -D-glucuronopyranoside	Leaves	Flavones	-	Yang et al 2016
60.	Tricin 7- <i>O</i> -(6"- <i>O</i> -malonyl)- β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
61.	Tricin 7- <i>O</i> -(6"-(<i>E</i>)-sinapoyl)- β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
62.	Tricin 4'- <i>O</i> -(<i>threo</i> - β -syringylglyceryl) ether 7"- <i>O</i> - β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
63.	Tricin 4'- <i>O</i> -(<i>erythro</i> - β -guaiaacylglyceryl) ether	Bran	Flavones	DPPH red. sca. acti.	Ajitha et al 2012
64.	Tricin 4'- <i>O</i> -(<i>threo</i> - β -guaiaacylglyceryl) ether	Bran	Flavones	DPPH red. sca. acti.	Ajitha et al 2012
65.	Tricin 4'- <i>O</i> -(<i>erythro</i> - β -guaiaacylglyceryl) ether 7- <i>O</i> - β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
66.	Tricin 4'- <i>O</i> -(<i>threo</i> - β -guaiaacylglyceryl) ether 7- <i>O</i> - β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
67.	Tricin 4'- <i>O</i> -(<i>erythro</i> - β -guaiaacylglyceryl) ether 7"- <i>O</i> - β -D-glucopyranoside	leaves	Flavones	-	Yang et al 2016
68.	Tricin 4'- <i>O</i> -(<i>threo</i> - β -guaiaacylglyceryl) ether 7"- <i>O</i> - β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
69.	Tricin 4'- <i>O</i> -(<i>erythro</i> - β -guaiaacylglyceryl) ether 9"- <i>O</i> - β -D-glucopyranoside	Leaves	Flavones	-	Yang et al 2016
70.	Tricin 4'- <i>O</i> -(<i>threo</i> - β -4-hydroxyphenylglyceryl) ether	Leaves	Flavones	-	Yang et al 2016
71.	Tricin 7- <i>O</i> -rutinoside	Grains of brown rice	Flavones	-	Zeng et al 2019
72.	Brassicin	Grains of transgenic japonica	Flavonols	Redical scavenging activity	Cho et al 2013
73.	Brassicin-4'- <i>O</i> - β -D-glucopyranoside	Grains of transgenic japonica	Flavonols	Redical scavenging activity	Cho et al 2013
74.	Isorhamnetin-4'- <i>O</i> - β -D-glucopyranoside	Grains of transgenic japonica	Flavonols	Redical scavenging activity	Cho et al 2013
75.	Isorhamnetin-7- <i>O</i> - β -D-cellobioside	Grains of transgenic japonica	Flavonols	Redical scavenging activity	Cho et al 2013
76.	Kaempferol	Husk and Bran	Flavonols	-	Ding et al. 2019
77.	Myricetin	Rice flour	Flavonols	-	Irakli et al 2012
78.	Quercetin	Rice flour	Flavonols	-	Irakli et al 2012

79.	Quercetin 3- <i>O</i> -glucoside	Rice flour	Flavonols	-	Irakli et al 2012
80.	Quercetin 3- <i>O</i> -galactoside = Hyperoside	Rice flour	Flavonols	-	Irakli et al 2012
81.	Quercetin 3- <i>O</i> -rutinoside = Rutin	Rice flour	Flavonols	-	Irakli et al 2012
82.	Syringetin 3- <i>O</i> - β -D-glucopyranoside	Leaves	Flavonols	-	Yang et al 2016
83.	Naringenin	Leaves	Flavanones	-	Katsumata et al 2017
84.	Syringetin 3- <i>O</i> -rutinoside	Leaves	Flavonols	-	Yang et al 2016
85.	3'- <i>O</i> -Methyltaxifolin	Grains of transgenic rice	Flavanonols	Radical sca. activity	Cho et al 2013
86.	3'- <i>O</i> -Methyltaxifolin-7- <i>O</i> - β -D-glucopyranoside	Grains of transgenic rice	Flavanonols	Radical sca. activity	Cho et al 2013
87.	3'- <i>O</i> -Methyltaxifolin-4'- <i>O</i> - β -D-glucopyranoside	Grains of transgenic rice	Flavanonols	Radical sca. activity	Cho et al 2013
88.	3'- <i>O</i> -Methyltaxifolin-5- <i>O</i> - β -D-glucopyranoside	Grains of transgenic rice	Flavanonols	Radical sca. activity	Cho et al 2013
89.	Catechin	Rice flour	Flavanols	-	Irakli et al 2012
90.	Epicatechin	Rice flour	Flavanols	-	Irakli et al 2012
91.	Cyanidin	Bran	Anthocyanins	-	Loypimai et al 2016
		Black rice kernels		Antioxidant activity	Hao et al 2015
92.	Cyanidin 3- <i>O</i> -gentiobioside	Bran	Anthocyanins	-	Tamura et al 2010
93.	Cyanidin 3- <i>O</i> -glucoside	Bran	Anthocyanins	-	Tamura et al 2010
94.	Cyanidin 3- <i>O</i> -rutinoside	Kenels	Anthocyanins	-	Hou et al 2013
95.	Cyanidin 3- <i>O</i> -sambubioside	Black rice kernels	Anthocyanins	Antioxidant activity	Hao et al 2015
96.	Cyanidin 3,5- <i>O</i> -diglucoside	Kernels	Anthocyanins	-	Hou et al 2013
97.	Delphinidin	Bran	Anthocyanins	-	Loypimai et al 2016
98.	Malvidin	Bran	Anthocyanins	-	Loypimai et al 2016
99.	Pelargonidin	Bran	Anthocyanins	-	Loypimai et al 2016
100.	Pelargonidin 3,5- <i>O</i> -diglucoside	Pigmented rice	Anthocyanins	Antioxident activity	Dang et al 2013
101.	Peonidin	Black rice kernels	Anthocyanins	Antioxident activity	Hao et al 2015
102.	Peonidin 3- <i>O</i> -glucoside	Bran	Anthocyanins	-	Tamura et al 2010
103.	Camphene	Bran	Monoterpenoids	-	Chumpolsri et al 2015
104.	Camphor	Bran	Monoterpenoids	-	Chumpolsri et al 2015
105.	Carveol	Bran	Monoterpenoids	-	Chumpolsri et al 2015
106.	1,4-Cineol	Bran	Monoterpenoids	-	Chumpolsri et al 2015
107.	Fenchyl acetate	Bran	Monoterpenoids	-	Chumpolsri et al 2015
108.	(<i>S</i>)-Limonene	Leaves	Monoterpenoids	-	Obara et al 2002
		Seedlings		Antibact. act on <i>Xoo</i>	Lee et al 2016
109.	Linalool	Leaves	Monoterpenoids	Resistance induction to <i>Xoo</i>	Taniguchi et al 2014
110.	<i>cis</i> -Linalool oxide	Bran	Monoterpenoids	-	Chumpolsri et al 2015
111.	<i>trans</i> -Linalool oxide	Bran	Monoterpenoids	-	Chumpolsri et al 2015
112.	Myrcene	Seedlings	Monoterpenoids	-	Lee et al 2016
113.	<i>trans</i> - β -Ocimene	Bran	Monoterpenoids	-	Chumpolsri et al 2015
114.	α -Pinene	Seedlings	Monoterpenoids	-	Lee et al 2016
115.	β -Pinene	Bran	Monoterpenoids	-	Chumpolsri et al 2015
116.	Sabinene	Seedlings	Monoterpenoids	-	Lee et al 2016
117.	α -Terpinene	Seedlings	Monoterpenoids	-	Lee et al 2016
118.	γ -Terpinene	Leaves	Monoterpenoids	Antibact. act on <i>Xoo</i>	Yoshitomi et al 2016
119.	Terpinen-4-ol	Bran	Monoterpenoids	-	Chumpolsri et al 2015
120.	α -Thujene	Seedlings	Monoterpenoids	-	Lee et al 2016
121.	Abscisic acid	Whole rice plants	Sesquiterpenoids	Regulation of growth and development	Changan et al 2018
122.	(<i>Z</i>)- α -Bergamotene	Leaves	Sesquiterpenoids	-	Obara et al 2002
123.	β - Bisabolene	Bran	Sesquiterpenoids	-	Chumpolsri et al 2015
124.	(<i>E</i>)- γ -Bisabolene	Leaves	Sesquiterpenoids	-	Obara et al 2002
125.	α -Cadinene	Leaves	Sesquiterpenoids	-	Obara et al 2002
126.	β -Caryophyllene	Leaves	Sesquiterpenoids	-	Obara et al 2002

127.	α -Copaene	Leaves	Sesquiterpenoids	-	Obara et al 2002
128.	α -Curcumene	Leaves	Sesquiterpenoids	-	Obara et al 2002
129.	γ -Curcumene	Leaves	Sesquiterpenoids	-	Obara et al 2002
130.	Cyclosativene	Seedlings	Sesquiterpenoids	-	Lee et al 2016
131.	α -Elemene	Bran	Sesquiterpenoids	-	Chumpolsri et al 2015
132.	(<i>E</i>)- β -Farnesene	Leaves	Sesquiterpenoids	-	Kiryu et al 2018
133.	Germacrene D	Leaves	Sesquiterpenoids	-	Obara et al 2002
134.	α -Gurjunene	Bran	Sesquiterpenoids	-	Chumpolsri et al 2015
135.	β -Gurjunene	Leaves	Sesquiterpenoids	-	Obara et al 2002
136.	α -Humulene	Leaves	Sesquiterpenoids	-	Obara et al 2002
137.	β -Elemene	Seedlings	Sesquiterpenoids	-	Lee et al 2016
138.	Italicene	Leaves	Sesquiterpenoids	-	Obara et al 2002
139.	γ -Muurolole	Leaves	Sesquiterpenoids	-	Obara et al 2002
140.	(<i>E</i>)-Nerolidol	Leaves	Sesquiterpenoids	Antibacterial activity against <i>Xoo</i>	Kiryu et al 2018
141.	7- <i>epi</i> - α -Selinene	Bran	Sesquiterpenoids	-	Chumpolsri et al 2015
142.	Valencene	Leaves	Sesquiterpenoids	-	Obara et al 2002
143.	Viridiflorene	Leaves	Sesquiterpenoids	-	Obara et al 2002
144.	α -Ylangene	Bran	Sesquiterpenoids	-	Chumpolsri et al 2015
145.	α -Zingiberene	Leaves	Sesquiterpenoids	-	Obara et al 2002
146.	Momilactone A	Coleoptiles Root exudates	Diterpenoids	Antifungal activity Allelopathy effect	Cartwright et al 1981 Kato-Noguchi et al 2008
147.	Momilactone B	Coleoptiles Root exudates	Diterpenoids	Antifungal activity Allelopathy effect	Cartwright et al 1981 Kato-Noguchi et al 2008
148.	Momilactone C	Bran	Diterpenoids	-	Tsunakawa et al 1976
149.	Momilactone D	Roots	Diterpenoids	-	Cho et al 2015
150.	Momilactone E	Roots	Diterpenoids	-	Cho et al 2015
151.	9 β -Pimara-7,15-diene- 3 β ,6 β ,19-triol	Leaves	Diterpenoids	Weak fungal activity	Horie et al 2015
152.	<i>ent</i> -15,16-Epoxy-2,3- dihydroxy- kaurane	Leaves of a bacterial leaf blight-resistant cultivar	Diterpenoids	Antibacterial activity	Watanabe et al 1992
153.	<i>ent</i> -2,3,15-Trihydroxy- kaurane	Leaves of a bacterial leaf blight-resistant cultivar	Diterpenoids	Antibacterial activity	Watanabe et al 1992
154.	<i>ent</i> -15,16-Epoxy-kauran-3- one	Leaves of a bacterial leaf blight-resistant cultivar	Diterpenoids	Antibacterial activity	Watanabe et al 1992
155.	<i>ent</i> -15,16-Epoxy-kauran-2,3- dione = Oryzadione	Leaves of a bacterial leaf blight-resistant cultivar	Diterpenoids	Antibacterial activity	Kono et al 2004
156.	<i>ent</i> -15,16-Epoxy-3 β - hydroxy-kauran-2-one	Leaves of a bacterial leaf blight-resistant cultivar	Diterpenoids	Antibacterial activity	Kono et al 2004
157.	<i>ent</i> -15,16-Epoxy-3-oxa- kauran-2-one	Leaves of a bacterial leaf blight-resistant cultivar	Diterpenoids	Antibacterial activity	Kono et al 2004
158.	<i>ent</i> -15,16-Epoxy-3 β - myristoyloxy-kauran-2-one	Leaves of a bacterial leaf blight-resistant cultivar	Diterpenoids	Antibacterial activity	Kono et al 2004
159.	<i>ent</i> -15,16-Epoxy-3 α - palmitoyloxy-kauran-2-one	Leaves of a bacterial leaf	Diterpenoids	Antibacterial activity	Kono et al 2004

160.	<i>ent</i> -15,16-Epoxy-3 β -palmitoyloxy-kauran-2-one	blight-resistant cultivar Leaves of a bacterial leaf blight-resistant cultivar	Diterpenoids	Antibacterial activity	Kono et al 2004
161.	Oryzalexin A	Leaves	Diterpenoids	Inhibitory activity on spore germination and germ tube growth of <i>Ochrobacterium oryzae</i>	Akatsuka et al 1998 Kono et al 1985
162.	Oryzalexin B	Leaves	Diterpenoids	Inhibitory activity on spore germination and germ tube growth of <i>O. oryzae</i>	Akatsuka et al 1985 Kono et al 1985
163.	Oryzalexin C	Leaves	Diterpenoids	Inhibitory activity on spore germination and germ tube growth of <i>O. oryzae</i>	Akatsuka et al 1985 Kono et al 1985
164.	Oryzalexin D	Leaves	Diterpenoids	Inhibitory activity on spore germination and germ tube growth of <i>M. oryzae</i>	Sekido et al 1986
165.	Oryzalexin E	Leaves	Diterpenoids	Inhibitory activity on spore germination and germ tube growth of <i>M. oryzae</i>	Kato et al 1993
166.	Oryzalexin F	Leaves	Diterpenoids	Antimicrobial activity	Kato et al 1994
167.	Oryzalic acid A	Leaves of a bacterial leaf Blight-resistant cultivar	Diterpenoids	Antibacterial activity	Kono et al 1991
168.	Oryzalic acid B = <i>ent</i> -15-Hydroxy-2,3-secokauren-2,3-dioic acid	Leaves of bacterial leaf Blight resistant cultivar	Diterpenoids	Antibacterial activity	Watanabe et al 1992
169.	Oryzalide A = <i>ent</i> -15,16-Epoxy-1 α -hydroxy-2-oxa-kauran-3-one	Leaves of bacterial leaf Blight resistant cultivar	Diterpenoids	Antibacterial activity	Watanabe et al 1990 Kono et al 1991
170.	Oryzalide B	Leaves of bacterial leaf Blight resistant cultivar	Diterpenoids	Antibacterial activity	Kono et al 1991
171.	Sandaracopimaradien-3-one	Roots	Diterpenoids	-	Cho et al 2015
172.	Oryzalexin S	Leaves	Diterpenoids	Antifungal activity	Kodama et al 1992 Tamogani et al 1993
173.	Stemar-13-en-2 α -ol	Leaves	Diterpenoids	Weak antifungal activity	Horie et al 2015
174.	Phytocassane A	Leaves infected with <i>M. oryzae</i> ; stems infected with Rhizoctoniasolani	Diterpenoids	Antifungal activity	Koga et al 1995
175.	Phytocassane B	Leaves infected with <i>M. oryzae</i> ; Stem infected with <i>R. solani</i>	Diterpenoids	Antifungal activity	Koga et al 1995
176.	Phytocassane C	Leaves infected	Diterpenoids	Antifungal activity	Koga et al 1995

		with <i>M. oryzae</i> ; Stem infected with <i>R. solani</i>			
177.	Phytocassane D	Leaves infected with <i>M. oryzae</i> ; Stem infected with <i>R. solani</i>	Diterpenoids	Antifungal activity	Koga et al 1995
178.	Phytocassane E	Cultured rice cells	Diterpenoids	Inhibition activity on spore germination and germ tube growth of <i>M. oryzae</i>	Koga et al 1997
179.	Phytocassane F	Leaves	Diterpenoids	Antifungal activity	Horie et al 2015
180.	5-Deoxy- <i>ent</i> -10- oxodepressin	Leaves	Diterpenoids	Antifungal activity	Horie et al 2016
181.	5-Dihydro- <i>ent</i> -10- oxodepressin	Leaves	Diterpenoids	Antifungal activity	Horie et al 2016
182.	<i>ent</i> -10-Oxodepressin	Leaves	Diterpenoids	Antifungal activity	Inoue et al 2013
183.	Citrostadienol	Bran	Triterpenoid	- Anti-inflammatory activity	Verardo et al 2016 Akihisa et al 2000
184.	Citrostadienol <i>cis</i> -ferulate	Bran	Triterpenoid	Anti-inflammatory activity	Akihisa et al 2000
185.	Citrostadienol <i>trans</i> -ferulate	Bran	Triterpenoid	Anti-inflammatory activity	Akihisa et al 2000
186.	(24 <i>S</i>)-Cycloart-25-ene- 3 β ,24-diol-3 β - <i>trans</i> -ferulate	Bran	Triterpenoid	Moderate cytotoxic activity	Luo et al 2005
187.	Cycloartenol	Bran	Triterpenoid	-	Verardo et al 2016
188.	Cycloartenol <i>trans</i> -caffeate	Seeds	Triterpenoid	-	Shu et al 2008
189.	Cycloartenol <i>cis</i> -ferulate	Bran	Triterpenoid	-	Fang et al 2003
190.	Cycloartenol <i>trans</i> -ferulate	Bran	Triterpenoid	-	Fang et al 2003
191.	24-Methylene cycloartanol	Bran of black non- glutinous rice	Triterpenoid	Anticancer activity	Suttiarporn et al 2015
192.	24-Methylene cycloartanol <i>trans</i> -ferulate	Bran	Triterpenoid	-	Fang et al 2003
193.	Cycloeucalenol	Bran of black non- glutinous rice	Triterpenoid	Anti-cancer activity	Suttiarporn et al 2015
194.	Cycloeucalenol <i>cis</i> -ferulate	Bran	Triterpenoid	Antioxidant activity	Wang et al 2015
195.	Cycloeucalenol <i>trans</i> -ferulate	Bran	Triterpenoid	-	Fang et al 2003 Akihisa et al 2000 Wang et al 2015
196.	Gramisterol	Bran of black non- glutinous rice	Triterpenoid	Anti-cancer activity	Suttiarporn et al 2015
197.	Gramisterol <i>cis</i> -ferulate	Bran	Triterpenoid	Anti-inflammatory activity	Akihisa et al 2000
198.	Gramisterol <i>trans</i> -ferulate	Bran	Triterpenoid	Anti-inflammatory activity	Akihisa et al 2000
199.	Lanast-7,9(11)-dien-3 α ,15 α - diol-3 α -D-glucofuranoside	Hulls	Triterpenoid	Herbicidal activity	Chung et al 2006
200.	1-phenyl-2-hydroxy-3,7- dimethyl-11-aldehydic- tetradecane-2 β -D- glucopyranoside	Hulls	Other	Herbicidal activity	Chung et al 2006
201.	stigmastanol-3 β -p- butanoxydihydrocoumaroate	Hulls	Steroids	Weak inhibitory effect towards duckweed (<i>Lemna paucicostata</i>)	Chung et al 2006
202.	stigmastanol-3 β -p- glyceroxydihydrocoumaroat e	Hulls	Steroids	-	Chung et al 2006
203.	Lupeol	Bran of black non- glutinous rice	Triterpenoid	Anticancer activity	Suttiarporn et al 2015

204.	Lupenone	Bran of black non-glutinous rice	Triterpenoid	Anticancer activity	Suttiarporn et al 2015
205.	<i>N</i> -Feruloylagmatine	Leaves	Alkaloids	Antimicrobial activity	Morimoto et al 2018
206.	<i>N</i> -Feruloylputrescine	Leaves	Alkaloids	Antimicrobial activity	Morimoto et al 2018
207.	Kynurenic acid	Leaves	Alkaloids	-	Yang et al 2014
208.	Lycoperodine-1	Leaves	Alkaloids	-	Yang et al 2014
209.	2-Acetyl-1-pyrroline	Grains	Alkaloids	-	Buttery et al 1983
210.	<i>N</i> -Benzoylserotonin	Leaves	Alkaloids	Antibacterial activity	Morimoto et al 2018
211.	<i>N</i> -Benzoyltryptamine	Leaves	Alkaloids	Antimicrobial activity	Morimoto et al 2018
212.	<i>N</i> -Benzoyltyramine	Leaves	Alkaloids	Antimicrobial activity	Morimoto et al 2018
213.	<i>N-trans</i> -Cinnamoylserotonin	Leaves	Alkaloids	Antimicrobial activity	Morimoto et al 2018
214.	<i>N-trans</i> -Cinnamoyltryptamine	Leaves	Alkaloids	Antimicrobial activity	Morimoto et al 2018
215.	<i>N-trans</i> -Cinnamoyltyramine	Whole rice plant Leaves	Alkaloids	Allelopathic activity Antifungal activity Antibacterial activity	Park et al 2014 Le et al 2014 Park et al 2014
216.	<i>N-p</i> -Coumaroylserotonin	Leaves	Alkaloids	Antibacterial activity	Morimoto et al 2018
217.	<i>N</i> -Feruloylserotonin	Leaves	Alkaloids	Antibacterial activity	Morimoto et al 2018
218.	<i>N</i> -Feruloyltryptamine	Leaves	Alkaloids	-	Ishihara et al 2008
219.	Indole 3-acetic acid	Whole rice plant	Alkaloids	Regulation of growth and development	Yamamoto et al 2007
220.	Serotonin = 5-Hydroxytryptamine	Leaves	Alkaloids	-	Ishihara et al 2008
221.	Tryptamine	Leaves	Alkaloids	-	Ishihara et al 2008
222.	(<i>E,E</i>)-2,4-Heptadienal	Whole plants	Other	Antibacterial, Antifungal activity	Tanaka et al 2014
223.	(<i>Z</i>)-3-Hexen-1-ol	Leaves	Other	-	Obara et al 2002
224.	Orizaanthracenol = 1-Methoxyanthracen-2-ol	Hulls	Others	Strong inhibitory activity in seed germination in radish	Chung et al 2006
225.	<i>cis</i> -12-oxo-Phytodienoic acid	Whole plants	Others	Inducible anti-insect activity	Guo et al 2014
226.	1-Phenyl-2-hydroxy-3,7-dimethyl-11-aldehydic-tetradecane-2 β -D-glucopyranoside	Hulls	Others	Herbicidal activity	Chung et al 2006
227.	(5 <i>S</i>)-5-(Acetyloxy)-3-(1-methylentyl)-2-cyclohexen-1-one = 3-Isopropyl-5-acetoxycyclohexene-2-one-1	Leaves	Others	Allelopathic activity	Kong et al 2004
228.	α -Tocopherol	Bran	Other	Antioxidative, anticancer	Sookwong et al 2009
229.	β -Tocopherol	Bran	Other	Antioxidative, anticancer	Sookwong et al 2009
230.	γ -Tocopherol	Bran	Other	Antioxidative, anticancer	Sookwong et al 2009
231.	δ -Tocopherol	Bran	Other	Antioxidative, anticancer	Sookwong et al 2009
232.	α -Tocotrienol	Bran	Other	Antioxidative, anticancer	Sookwong et al 2009
233.	β -Tocotrienol	Bran	Other	Antioxidative, anticancer	Sookwong et al 2009
234.	γ -Tocotrienol	Bran	Other	Antioxidative, anticancer	Sookwong et al 2009
235.	δ -Tocotrienol	Bran	Other	Anticancer	Sookwong et al 2009

Table S2 — Blind Docking based selected phytochemical compounds for the docking of three consecutive active sites.

S.No	Compound Name	PubChem CID	Lead ID	Binding Score Active site Docking			Average Binding Score
				Score 1	Score 2	Score 3	
1	Syringaldehyde	8655	lead21	-5.7	-5.7	-5.7	-5.70
2	Catechin	9064	lead22	-7.6	-7.6	-7.6	-7.60
3	Syringic acid	10742	lead24	-6.1	-6.1	-6.1	-6.10
4	α -Tocopherol	14985	lead27	-7.3	-7.5	-7.3	-7.37
5	2-Hydroxy 5-[(3S)-3-hydroxybutyl] phenyl β -D-glucoside (HHPG)	171378361	lead32	-7.5	-7.4	-7.5	-7.46
6	Epicatechin	72276	lead33	-7.5	-7.5	-7.5	-7.50
7	δ -Tocopherol	92094	lead36	-7.2	-7.3	-7.3	-7.27
8	γ -Tocopherol	92729	lead40	-7.5	-7.7	-8	-7.73
9	Delphinidin	128853	lead45	-7.2	-7.2	-7.2	-7.20
10	Cyanidin	128861	lead46	-7.1	-7.1	-7.1	-7.10
11	Pelargonidin	440832	lead57	-7.2	-7.2	-7.2	-7.20
12	Cyanidin 3-O-rutinoside	441674	lead58	-8	-8	-8	-8.00
13	Cyanidin 3,5-O-diglucoside	441688	lead59	-8	-8	-8	-8.00
14	Pelargonidin 3,5-O-diglucoside	441772	lead60	-8.6	-8.7	-8.7	-8.67
15	Peonidin	441773	lead61	-7.3	-7.3	-7.3	-7.30
16	Schaftoside	442658	lead64	-7.7	-7.6	-7.6	-7.63
17	N-Benzoyltyramine	577614	lead69	-7.4	-7.5	-7.4	-7.43
18	m-Coumaric acid	637541	lead71	-6.2	-6.2	-6.2	-6.20
19	Sinapic acid	637775	lead73	-6.2	-6.2	-6.2	-6.20
20	N-Benzoyl Tryptamine	684658	lead75	-7.4	-7.4	-7.5	-7.43
21	Isoschaftoside	3084995	lead81	-7.6	-7.8	-7.9	-7.77
22	Quercetin	5280343	lead82	-7.5	-7.5	-7.5	-7.50
23	1-O-Sinapoyl- β -D-glucose	5280406	lead83	-7	-7	-7	-7.00
24	Quercetin 3-O-glucoside	5280804	lead84	-7.8	-7.8	-7.8	-7.80
25	Rutin	5280805	lead85	-8	-8	-8	-8.00
26	Kaempferol	5280863	lead86	-7.4	-7.3	-7.3	-7.33
27	(E)-Nerolidol	5281525	lead91	-6.1	-6.1	-6.1	-6.10
28	Hyperoside	5281643	lead93	-7.9	-7.9	-7.9	-7.90
29	Myricetin	5281672	lead94	-7.6	-7.6	-7.6	-7.60
30	Tricin	5281702	lead95	-7.7	-7.7	-7.7	-7.70
31	N-FeruloylPutrescine	5281796	lead96	-6.4	-6.4	-6.4	-6.40
32	Cycloartenol trans-ferulate	5282164	lead97	-8.5	-8.5	-8.5	-8.50
33	β -Tocotrienol	5282348	lead98	-8.1	-8.3	-8.3	-8.23
34	γ -Tocotrienol	5282349	lead99	-7.4	-8.3	-7.7	-7.80
35	δ -Tocotrienol	5282350	lead100	-7.8	-7.8	-7.6	-7.73
36	(E,E)-2,4-Heptadienal	5283321	lead101	-4.6	-4.5	-4.6	-4.57
37	(E)-Nerolidol	5284507	lead103	-6.2	-6.2	-6.2	-6.20
38	N-trans-CinnamoylTyramine	5315911	lead104	-7.5	-7.4	-7.4	-7.43
39	3-O-Feruloylquinic acid	5317346	lead105	-7.3	-7.3	-7.3	-7.30
40	Syringetin 3-O- β -D- glucopyranoside	5321577	lead107	-8.9	-8.9	-8.9	-8.90
41	N-Feruloyltryptamine	5458878	lead113	-8.4	-8.4	-8.4	-8.40
42	N-p-Coumaroylserotonin	5458879	lead114	-8	-8.1	-7.6	-7.90
43	N-Feruloyl Serotonin	5969616	lead116	-8.1	-7.6	-8	-7.90
44	3-O-p-Coumaroyl quinic acid	6441280	lead120	-7.4	-7.5	-7.5	-7.47
45	3-O-Feruloylquinic acid	6451331	lead122	-7.4	-7.5	-7.4	-7.43
46	Brassicin	6455477	lead123	-8.1	-8.1	-8.1	-8.10

47	Cyanidin 3-O-sambubioside	6602304	lead124	-8	-8	-7.9	-7.97
48	β -Tocopherol	6857447	lead125	-7.2	-7.3	-7.3	-7.27
49	3-O-Feruloylquinic acid	9799386	lead127	-7.9	-7.9	-8.1	-7.97
50	N-trans-Cinnamoyl Serotonin	9995324	lead130	-8.3	-8.2	-8.3	-8.27
51	3-O-Feruloylquinic acid	10133609	lead133	-7.2	-7.2	-7.1	-7.17
52	(E)-Nerolidol	11241545	lead141	-6.2	-6.2	-6.2	-6.20
53	Cyanidin 3-O-gentiobioside	11968393	lead144	-8.4	-8.4	-8.3	-8.37
54	Isorhamnetin-4'-O- β -D-glucopyranoside	11968470	lead145	-8.3	-8.3	-8.3	-8.30
55	γ -Curcumene	12304273	lead148	-6.3	-6.3	-6.3	-6.30
56	1-O-Feruloyl- β -D-glucose	13962928	lead151	-7.5	-7.5	-7.5	-7.50
57	1,3-O-Diferuloylglycerol	14135369	lead152	-7.4	-7.4	-7.3	-7.37
58	p-Hydroxy methyl benzoate glucoside	15139313	lead154	-7.2	-7.2	-7.2	-7.20
59	Syringetin 3-O- β -D-glucopyranoside	20056942	lead158	-7.5	-7.5	-7.5	-7.50
60	Tricin 4' -O-(threo- β -guaiacylglyceryl) ether	21575482	lead160	-7.8	-8.1	-8.1	-8.00
61	Isoorientin 7,3' -dimethyl ether	25002956	lead163	-7.5	-7.5	-7.5	-7.50
62	Tricin 7-O-rutinoside	44258273	lead167	-8.2	-8.2	-8.2	-8.20
63	Tricin 5-O- β -D-glucopyranoside	49800176	lead172	-7.6	-7.6	-7.6	-7.60
64	Tricin 7-O-(6" -(E)-sinapoyl)- β -D-glucopyranoside	71728409	lead174	-7.9	-8	-8	-7.97
65	3-O-Feruloylquinic acid	73210496	lead175	-7.1	-7.1	-7.1	-7.10
66	Tricin 4' -O-(erythro- β -guaiacylglyceryl) ether	101193641	lead184	-8	-7.9	-8	-7.97
67	Tricin 4'-O-(threo- β -guaiacylglyceryl) ether)7-O- β -D-glucopyranoside	101193642	lead185	-7.9	-8.2	-7.8	-7.97
68	Syringetin 3-O-rutinoside	101552528	lead186	-7.5	-7.5	-7.5	-7.50
69	tricin 7-O-neohesperidoside	102158614	lead191	-8.4	-8.4	-8.4	-8.40
70	Tricin 4'-O-(erythro- β -guaiacylglyceryl) ether 7" -O- β -D-glucopyranoside	122376001	lead197	-7.5	-7.8	-7.9	-7.73
71	Apigenin 6-C- α -L-arabinosyl-8-C- β -L-arabinside	122391239	lead200	-7.2	-7.2	-7.2	-7.20
72	Tricin 7-O-(6"-O-malonyl)- β -D-glucopyranoside	122391240	lead201	-8.8	-8.1	-8.8	-8.57
73	luteolin 6-C-(2" -O- β -D-glucopyranosyl)- α -L-arabinside	131750830	lead203	-7.9	-7.8	-7.8	-7.83
74	Abscisic acid	131954763	lead212	-6.8	-7.1	-6.9	-6.93
75	N-Feruloylagmatine	132280331	lead216	-7.2	-6.6	-6.7	-6.83
76	Helvolic acid	139588222	lead220	-8.3	-8.4	-8.3	-8.33
77	Cyanidin 3-O-glucoside	441667	lead223	-8.5	-8.5	-8.4	-8.47
78	Peonidin 3-O-glucoside	443654	lead226	-8.6	-8.6	-8.6	-8.60
79	Chrysoeriol 7-O-rutinoside	14374725	lead230	-8.4	-8.5	-8.6	-8.50
80	Isoscoparin 2-O-(6-(E)-feruloyl)-glucopyranoside	21722000	lead232	-9	-9	-8.9	-8.97
81	Isoscoparin 2" -O-(6" -(E)-p-coumaroyl)-glucopyranoside	21722001	lead233	-8.1	-8.1	-8.1	-8.10
82	Isovitexin 2" -O-(6" -(E)-p-coumaroyl)-glucopyranoside	44257727	lead234	-7.7	-7.7	-7.8	-7.73
83	Isovitexin 2" -O-(6" -(E)-feruloyl)-glucopyranoside	44257728	lead235	-8.2	-8.2	-8.2	-8.20