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Compound	Category	Subcategory	Origin	Function	Reference
			(Either general or		
			specific plants		
			reported)		
Linalool (1)		Monoterpene	Penstemon	1) Slow the growth rate of phyllosphere origin bacterial	31
			digitalis	strains.	
				2) Promote the maximum density of nectary-source	
				bacterial groups.	
β -Caryophyllene (2)		Sesquiterpene	Arabidopsis	1) Protect the Arabidopsis floral organ from	32
			thaliana;	Pseudomonas syringae pv tomato DC3000.	
			tomato	2) Shift the root microbiota composition of neighboring	
			(Solanum	tomato plants.	
	Terpene		lycopersicum)		
Capsidiol (3)		Sesquiterpene	Pepper and	1) Act as a phytoalexin in response to pathogens	33
			tobacco	including the potato late blight causer Phytophthora	
				infestans.	
Kauralexin A1 (4)		Diterpene	Maize	1) Confer maize plants with tolerance of	36–38
Kauralexin B1 (5)		-		phytopathogenic microbes such as Fusarium spp.,	
				Aspergillus spp., Collectotrichum spp, Rhizopus	
				microspores, and Cochliobolus heterostrophus.	
Epoxydolabrene (6)		Diterpene	Maize	1) Inhibit Fusarium verticillioides and Fusarium	37, 39
Epoxydolabrranol (7)		-		graminearum.	
Trihydroxydolabrene (8)				2) Modulate rhizosphere microbiome with pronounced	
				change of Alphaproteobacteria.	
Momilactone A (9)		Diterpene	Rice	1) Respond to fungal signals e.g., chitin.	41-45
Momilactone B (10)				2) Protect plant from rice blast caused by <i>Magnaporthe</i>	
				oryzae.	
				3) Display <i>in vitro</i> antibacterial activities against	
				Bacillus pumilus, Pseudomonus ovalis, Escherichia	
				coli, and Bacillus cereus.	
Phytocassane A (11)		Diterpene	Rice	1) Suppress pathogenic microbes such as <i>Pyricularia</i>	40
Phytocassane B (12)				oryzae, Magnaporthe grisea and Magnaporthe oryzae.	
Oryzalexin A (13)		Diterpene	Rice		
Oryzalexin B (14)					
5,10-Diketo-casbene (15)		Diterpene	Rice japonica	1) Offer plants bacterial blight resistance by inhibiting	19,46,47
			varieties	<i>M. oryzae</i> spore germination.	

Supplementary Table 1. Origin and bioactivity of plant signaling metabolites.

				2) Alleviate leaf disease symptoms caused by the <i>Xoo</i>	
	_	Diterret	D a su las	strain.	4.9
Hordetriene (16)		Diterpene	Barely	1) Synthesis upon infections by bacterial and lungal	48
(17)				pathogen not beneficial lungus.	
(17) Debudreehisting1 (19)	_	Ditamana	Conifor	1) A stivute systemic acquired resistance for terrete	50
Denydroabletinal (18)		Diterpene	Conner	tobacco, and <i>A. thaliana</i> .	50
ent-Quiannulatene (19)	_	Sesterterpene	A. thaliana	1) Reshape the composition of root microbiota, with	52
Astellatene (20)	-	Sesterterpene	A. thaliana	changes of OTUs of Firmicutes, Proteobacteria,	
		•		Actinobacteria, Planctomycetes, Verrucomicrobita, and	
				Acidobacteria.	
Thalianin (21)		Triterpene	A. thaliana	1) Modulate the assembly of <i>A. thaliana</i> root bacterial	18
Arabidin (22)	_	Triterpene	A. thaliana	microbiota, sustaining Arenimonas proliferation and	
		_		suppressing Arthrobacter growth.	
Avenacin A1 (23)		Triterpene	Oat	1) Provide plants with resistance to "take-all" caused	53-55
Avenacin B1 (24)				by fungus Gaeumannomyces tritici.	
				2) Structure oat-associated rhizosphere eukaryotes.	
Ginsenoside Rg1 (25)		Triterpene	Panax	1) Drive <i>Panax notoginseng</i> associated soil microbiota.	56
Ginsenoside Rb1 (26)			notoginseng		
Ginsenoside Rd (27)					
Orobanchol (28)		Higher-terpene	various	1) Establish plant-AMF association.	57-62
5-Deoxystrigol (29)			monocotyledonous	2) Steer rice plant rhizomicrobiome and promote	
Carlacton (30)			and	beneficial bacteria.	
Carlactonoic acid (31)			dicotyledonous	3) Alter soybean rhizosphere microbial compositions.	
Lotuslactone (32)			plants, e.g., rice,	4) Change sorghum rhizosphere bacterial groups.	
			soybean, and		
			sorghum		
Sakuranetin (33)		Flavonoid	Rice	1) Accumulate upon <i>Pyricularia oryzae</i> and	40
	Phenylpropanoid			Magnaporthe grisea attack.	
Glyceollin I (34)		Flavonoid	Soybean	1) Serve as phytoalexins in response to fungi	65–67
Glyceollin III (35)				Aspergillus species, and Rhizopus microspores var.	
				oryzae.	
Medicarpin (36)		Flavonoid	Medicago	1) Act as a phytoalexin in response to fungus <i>Phoma</i>	
				medicaginis.	
Maackiain (37)		Flavonoid	Chickpea	1) Induced synthesis by elicitor k-carrageenan.	
Pisatin (38)		Flavonoid	Pea	1) Produced upon pathogen Nectria haematococca	
				MPVI infection.	
				2) Induced synthesis by elicitor k-carrageenan.	

Apigenin (39)		Flavonoid	A range of legume plants and maize	 Induce host nodulation and establish plant-rhizobia symbiotic connection. Respond to infection by fungus <i>Colletotrichum</i> <i>graminicola</i> in maize plants. Coordinate maize-special rhizosphere microorganisms, enriching <i>Massilia</i> genus and <i>Oralobacteraceae</i> family 	13,68
				4) Enhance plant filed performance.	
Daidzein (40) Genistein (41)		Flavonoid	Legumes, e.g., soybean	1) Trigger soybean- <i>Bradyrhizobium</i> and legume- <i>Rhizobium</i> sp. NGR234 symbiosis but repress several <i>Rhizobium</i> strains.	68
Scopoletin (42)		Coumarin	A. thaliana	 Shape rhizomicrobiome, sustain beneficial microbes such as bacterium <i>P. simiae</i> WCS417 <i>P. capeferrum</i> WCS358 but repressing pathogenic fungi <i>F. oxysporum</i> and <i>V. dahlia</i>. Sculpt the assembly of microbiome, enriching <i>Pseudomonas</i> species. 	22
Fraxetin (43)		Coumarin	A. thaliana	1) Alter the root microbiota and enhance plant growth under iron-restricted condition, selecting iron- beneficial commensal strains.	71
Daphnetin (44)		Coumarin	Different plant sources	1) Inhibit phytopathogenic microbes such as <i>R</i> . <i>solanacearum</i> .	72
Resveratrol (45)		Stilbene	Vitaceae plants	1) Respond to fungal attacks from <i>B. cinerea</i> , <i>P. viticola</i> and <i>U. necator</i> .	74
Pterostilbene (46)		Stilbene	Vitaceae plants	1) Enhance plant resistance to the pathogen <i>Rhizoctonia solani</i> and reduce root necrosis in pterostilbene-expressed soybeans.	76,77
ε-Viniferin (47)		Stilbene	Vitaceae plants	1) Accumulate upon infection by <i>Plasmopara viticola</i> and <i>Erysiphe necator</i> .	75
<i>p</i> -Coumaroyl-tyramine (48)		Phenolamides	Pepper and others	1) Inhibit growth of pathogenic fungus Xanthomonas	78
<i>N</i> -feruloyl-tyramine (49)		Phenolamides	Oat	campestris.	70
Avenaninramide a (50)		Phenolamides	Oat	concentration-dependent manner.	/8
Cinnamoyltyramine (51)		Phenolamides	Rice	1) Protect plant against bacteria <i>Xoo</i> and fungus <i>Magnaporthe oryzae</i> along with phytoalexins synthesis.	82
Camalexin (52)		Alkaloid	Arabidopsis	1) Affect the rhizosphere microbiome.	24
Spirobrassinin (53)	N-containing	Alkaloid	Brassica rapa and	1) Respond to pathogens Albugo candida and	88,89

Rutalexin (54)	compound		Brassica juncea	Alternaria brassicola.	
Brassilexin (55)					
4-OH-ICN (56)		Cyanogenic compound	Arabidopsis	1) Maintain plant resistance to <i>P. syringae</i> pv. <i>tomato</i> DC3000.	21
				2) Inhibit growth of fungi <i>Alternaria brassicicola</i> and	
				Botrytis cinerea.	
DIMBOA (57)		Benzoxazinoid	Poaceae family	1) Impede the growth of pathogenic <i>Staphylococcus</i>	94-98
MBOA (58)			plants, e.g., maize	aureus but promote PGP bacterium Pseudomonas	
HM_2BOA -Glc (59)				putida.	
				2) Tailor microbial communities in both aboveground	
				and belowground parts of plants.	
Zeaoxazolinone (60)		Benzoxazinoid		1) Possess antimicrobial properties against Aspergillus	95
				flavus and Candida albicans.	
Phenoxazine (61)		Benzoxazinoid		1) Display antibacterial activity in vitro.	99
				2) Contribute to the stability of microbial assemblage.	
Sulforaphane (62)		Glucosinolate	Brassicales plants	1) Inhibit <i>P. syringae</i> strains by interfering with	103
				microbial type III secretion system.	
2-Phenylethylisothiocyanate	S-containing	Glucosinolate	Brassicales plants	1) Control a pea disease via soil amendments or plant	105
(63)	compound			rotations via altering rhizosphere bacterial community.	
<i>p</i> -		Glucosinolate	Brassicales plants,	1) Shape rhizosphere microbiota.	106
Hydroxybenzylglucosinolate			e.g., Arabidopsis	2) Establish and maintain relationship between plants	
(64)				and endophytic fungi, e.g., Serendipita indica	
				3) Sustain beneficial microbe <i>Colletotrichum</i>	
				tofieldiae	
Indole glucosinolates, e.g.,		Glucosinolate	Arabidopsis	1) Contain the overgrowth of <i>Colletotrichum tofieldiae</i>	108
neoglucobrassicin (65)				fungus.	
				2) Enable the establishment of beneficial roles for	
		~		plants grown in phosphate-deficient conditions.	100
Alliin (66)		S-alkyl-	Alliaceae plants	1) Show antibacterial and antifungal properties against	109
		cysteine		Agrobacterium tumefaciens, Erwinia carotovora, P.	
		sulfoxides		syringae, Xanthomonas campestris, A. brassisicola, B.	
				cinerea, Magnaporthe grisea, Oomycete Phytophthora,	
	0.1		C1	Plectosphaerella cucumerina, among others.	1.5
Falcarindiol (67)	Other	Acetylenic	Slanaceous	1) Produced upon induction by <i>Cladosporium julvum</i> ,	15
		lany acids	species, e.g.,	2) Correlate with plant immunity with function P	
			iomato and	(2) Contracte with plant minimumity with lungus B.	
A avil sugars a g		A avl sugars	Component	1) Deduce tobacco specific funci (i.e. Eugerium and	122 122
Acyr sugars, e.g.,		Acyr sugars	Caryophynaceae,	1) Keduce tobacco specific fungi (i.e., <i>Fusarium</i> and	122, 123

S3:18(2,8,8) (68)	Geraniaceae,	Alternaria) spore germination.	
S3:17(2,7,8) (69)	Martyniaceae, and	2) Enhance protection from infection of	
	Solanaceae plants,	phytopathogens, B. cinerea and Pseudomonas	
	e.g., tobacco and	viridiflava when Arabidopsis treated with acyl	
	tomato	glycosides.	
		3) Induce soybean immunity against the disease target	
		spot.	
		4) Contribute to the formation of trichome-specific	
		microbiota.	
		5) Interplay between tomato plants and bacterial strain	
		Bacillus subtilis 3610.	