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SUPPLEMENTARY DATA

Supplementary Tables S1. List of the plant metabolites derived from PubChem and IMPPART database

PubChem CID	IMPPART ID	Name	Source
101289844	IMPHY002171	Kulolactone	*Azadirachta indica*
102090424	IMPHY010454	Vilasinin	*Azadirachta indica*
102146586	IMPHY004014	Azadirachtin	*Azadirachta indica*
10505484	IMPHY000150	Deacetylnimbin	*Azadirachta indica*
11119228	IMPHY000093	Nimbiol	*Azadirachta indica*
12004512	IMPHY002006	Gedunin	*Azadirachta indica*
12309055	IMPHY015072	beta-Sitosterol-beta-D-glucoside	*Abelmoschus moschatus*
12309449	IMPHY013093	delta-Elemene	*Acacia tortilis*
12313020	IMPHY011792	gamma-Muurolene	*Abies alba*
13875774	IMPHY002654	Nimbocinolide	*Azadirachta indica*
14458886	IMPHY011498	3- Deacetylsalannin	*Azadirachta indica*
14467538	IMPHY002857	28- Deoxonimbolide	*Azadirachta indica*
15560423	IMPHY001600	Kulactone	*Azadirachta indica*
177090	IMPHY012408	Nimbosone	*Azadirachta indica*
189706	IMPHY009443	Nimbionone	*Azadirachta indica*
189726	IMPHY013919	Margolonone	*Azadirachta indica*
68171	IMPHY007273	1-Hexacosanol	*Acacia concinna*
243696	IMPHY002935	1-Nonacosanol	*Aerva javanica*
222284	IMPHY014836	Beta-Sitosterol	*Abelmoschus esculentus*
25203368	IMPHY014396	Quercetin-3-glucoside	*Acacia leucophloea*
3034112	IMPHY014771	Deacetylgedunin	*Azadirachta indica*
31291	IMPHY003537	Tetredecanal	*Acinos alpinus*
42608158	IMPHY016012	Allo-Aromadendrene	*Acanthospermum hispidum*
44567124	IMPHY001446	Kulinone	*Azadirachta indica*
44715635	IMPHY001280	Nimbinene	*Azadirachta indica*
49863985	IMPHY011387	Epoxyazadiradione	*Azadirachta indica*
5280460	IMPHY011541	Scopoletin	*Adansonia digitata*
5280794	IMPHY014842	Stigmasterol	*Abelmoschus moschatus*
5280805	IMPHY015047	Rutin	*Abutilon theophrasti*

5281243	IMPHY011620	Lutein	*Allium cepa*
5281515	IMPHY014831	Beta-Caryophyllene	*Abelmoschus esculentus*
5281519	IMPHY005618	Germacrene B	*Acacia mearnsii*
5281520	IMPHY011761	Humulene	*Abies alba*
5281643	IMPHY014935	Hyperoside	*Abelmoschus esculentus*
5353609	IMPHY004432	Methyl 2,5-dihydroxycinnamate	*Azadirachta indica*
5742590	IMPHY014838	Sitogluside (Daucosterol)	*Abelmoschus moschatus*
6432312	IMPHY012921	gamma-Elemene	*Acacia mearnsii*
6918391	IMPHY010080	Beta-Elemene	*Abies nephrolepis*
6918774	IMPHY006612	Corosolic acid	*Actinidia eriantha*
71597391	IMPHY013522	triterpenoids	*Abelmoschus esculentus*
91886694	IMPHY007392	2',3'-Dehydrosalannol	*Azadirachta indica*
94162	IMPHY007375	Sugiol	*Azadirachta indica*
984	IMPHY007467	Hexadecanal	*Acalypha fruticosa*
19725	IMPHY015123	Alpha-Copaene	*Abelmoschus esculentus*
521710	IMPHY004521	Alpha-Patchoulene	*Achillea millefolium*
5281303	IMPHY014597	Azadirachtin A	*Azadirachta indica*
5280489	IMPHY011707	beta-Carotene	*Acacia decurrens*
-	IMPHY000464	Isomargosinolide	*Azadirachta indica*
101425842	IMPHY002244	Isoazadirolide	*Azadirachta indica*
76316558	IMPHY006017	Isomeldenin	*Azadirachta indica*
5281654	IMPHY008724	Isorhamnetin	Acacia catechu
-	IMPHY006786	Margosinolide	*Azadirachta indica*
177086	IMPHY006799	Meldenin	*Azadirachta indica*
100017	IMPHY000663	Methyl 2-[6-(furan-3-yl)-7	*Azadirachta indica*
44567123	IMPHY001448	Methyl kulonate	*Azadirachta indica*
5318767	IMPHY011985	Nicotiflorin	*Adiantum capillus-veneris*
108058	IMPHY012310	Nimbin	*Azadirachta indica*
189704	IMPHY005337	Nimbionol	*Azadirachta indica*
178770	IMPHY010224	Nimocinol	*Azadirachta indica*
12409	IMPHY009482	Nonacosane	*Acacia caven*
5280343	IMPHY004619	Quercetin	*Abelmoschus esculentus*
5280459	IMPHY015054	Quercitrin	*Abies pindrow*
5997	IMPHY006300	Cholesterol	*Abelmoschus moschatus*

Supplementary Tables S2. Molecular Docking result of plant metabolites with Vp9 (2GJI) protein of WSSV

Protein PDB ID	Ligand PubChem/IMPPART ID	Binding affinity (Kcal/mol)
2GJI	101289844	-6.6
	102090424	-7.3
	102146586	-5.8
	10505484	-5.9
	11119228	-6.6
	12004512	-7.1
	12309055	-6.4
	12309449	-4.7
	12313020	-5
	13875774	-6.8
	14458886	-6
	14467538	-5.9
	15560423	-6.9
	177090	-6.6
	189706	-6.9
	189726	-6.6
	68171	-3.4
	243696	-3.3
	222284	-6.6
	25203368	-6.4
	3034112	-7.4
	31291	-3.7
	42608158	-5.1
	44567124	-6.3
	44715635	-6
	49863985	-6.4
	5280460	-5.1
	5280794	-6.8
	5280805	-6.6
	5281243	-6.7
	5281515	-5.3
	5281519	-5.1
	5281520	-5.3
	5281643	-6.7
	5353609	-5
	5742590	-6.4
	6432312	-5.2
	6918391	-4.8
	6918774	-7.2
	71597391	-6.6
	91886694	-6
	94162	-6.4
	984	-3.3
	19725	-4.8
	521710	-4.9
	5281303	-6

	5280489	-6.5
	IMPHY000464	-6.3
	101425842	-6
	101425842	-6.3
	76316558	-5.9
	5281654	-6
	IMPHY006786	-6.4
	177086	-6.4
	100017	9
	44567123	-6.1
	5318767	-6.1
	108058	-5.6
	189704	-6.6
	178770	-7
	12409	-3.5
	5280343	-6
	5280459	-6.9
	5997	-6.2

Supplementary Table S3. Molecular docking result of plant metabolites with Vp26 protein (2EDM) of WSSV

Protein PDB ID	Ligand PubChem/IMPPART ID	Binding affinity (Kcal/mol)
2EDM	101289844	-6.5
	102090424	-6.3
	102146586	-6.3
	10505484	-5.9
	11119228	-6.8
	12004512	-6.5
	12309055	-6.7
	12309449	-4.7
	12313020	-5.4
	13875774	-6.1
	14458886	-6
	14467538	-6
	15560423	-6.3
	177090	-6.2
	189706	-6.3
	189726	-6.2
	68171	-3.1
	243696	-3
	222284	-6.5
	25203368	-7.7
	3034112	-6.7
	31291	-3.1
	42608158	-5.4
	44567124	-6.2
	44715635	-6.2

	49863985	-6.5
	5280460	-5.5
	5280794	-6.6
	5280805	-8.2
	5281243	-7
	5281515	-5.3
	5281519	-5.2
	5281520	-5.4
	5281643	-7.9
	5353609	-5
	5742590	-6.9
	6432312	-4.8
	6918391	-4.8
	6918774	-6.6
	71597391	-6.6
	91886694	-6.2
	94162	-6.3
	984	-3.1
	19725	-5.4
	521710	-6.1
	5281303	-7.2
	5280489	-7.1
	IMPHY000464	-6.3
	101425842	-6.6
	101425842	-6.5
	76316558	-8.1
	5281654	-7.2
	IMPHY006786	-6.3
	177086	-5.9
	100017	-6.1
	44567123	-7.1
	5318767	-6.6
	108058	-7.3
	189704	-6.3
	178770	-6
	12409	-8.1
	5280343	-8.9
	5280459	-8.3
	5997	-5.8

Supplementary Table S4: Molecular docking result of plant metabolites with Vp28 protein (2ED6) of WSSV

Protein PDB ID	Ligand PubChem/IMPPART ID	Binding affinity (Kcal/mol)
2ED6	101289844	-7.6
	102090424	-7.8
	102146586	-8.4
	10505484	-8

	11119228	-7.8
	12004512	-8.4
	12309055	-7.8
	12309449	-6.2
	12313020	-6.8
	13875774	-7.4
	14458886	-6.9
	14467538	-7.9
	15560423	-8.7
	177090	-6.9
	189706	-7.1
	189726	-7.5
	68171	-3.6
	243696	-3.4
	222284	-7.1
	25203368	-9.2
	3034112	-8.6
	31291	-4.6
	42608158	-6.8
	44567124	-7
	44715635	-6.8
	49863985	-8.2
	5280460	-6.8
	5280794	-7.4
	5280805	-8.3
	5281243	-7.4
	5281515	-6.6
	5281519	-6.5
	5281520	-6.5
	5281643	-9.6
	5353609	-6.2
	5742590	-7.7
	6432312	-6.1
	6918391	-6.2
	6918774	-9
	71597391	-8.5
	91886694	-6.6
	94162	-8.2
	984	-3.5
	19725	-5.6
	521710	-6.7
	5281303	-7.8
	5280489	-7.6
	IMPHY000464	-7.9
	101425842	-8.1
	101425842	-8.3
	76316558	-6.3
	5281654	-7.2

	IMPHY006786	-7.2
	177086	-6.9
	100017	9
	44567123	-7.1
	5318767	-7.9
	108058	-8
	189704	-7.5
	178770	-7.3
	12409	-3.2
	5280343	-7.7
	5280459	-7.5
	5997	-7.8