

Supplementary Materials

Exploring the Antibacterial Activity of *Pestalotiopsis* spp. under Different Culture Conditions and Their Chemical Diversity Using LC–ESI–Q–TOF–MS

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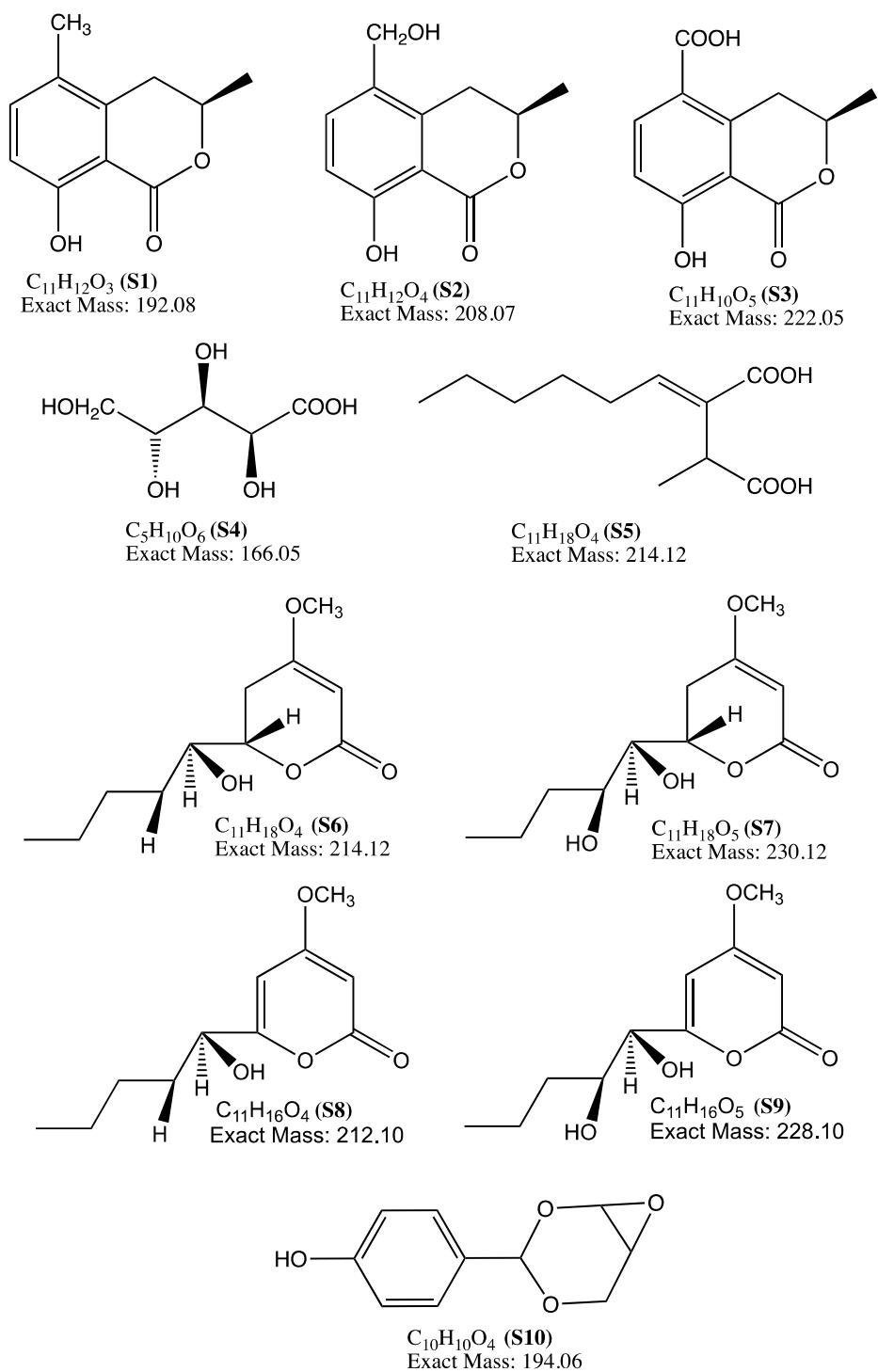


Figure S1: Structure compounds previously isolated from *P. mangiferae*. Compounds **S1-S9** were reported by Ortega et. al (2014) and compound **S10** by Subban et. al (2013).

Table S1. Culture parameters and amount of organic extract produced by *Pestalotiopsis* spp.

		Culture parameters			Amount of the organic extract (mg)			
Phase	Variation	Chemicals	pH	Temp. (°C)	<i>P. mangiferae</i>		<i>P. microspore</i>	
I	Chemicals	Arg	4.6 *	26	<i>man-1</i>	188.0	<i>mic-1</i>	86.0
		Glu			<i>man-2</i>	118.0	<i>mic-2</i>	100.0
		FeSO ₄			<i>man-3</i>	256.0	<i>mic-3</i>	251.0
		CaCl ₂			<i>man-4</i>	232.0	<i>mic-4</i>	297.0
		CuSO ₄			<i>man-5</i>	160.0	<i>mic-5</i>	329.0
II	pH	CaCl ₂	4.0	26	<i>man-6</i>	15.4	<i>mic-6</i>	157.0
		CaCl ₂	4.6		<i>man-7</i>	15.2	<i>mic-7</i>	127.1
		CaCl ₂	5.6		<i>man-8</i>	15.0	<i>mic-8</i>	32.7
		CuSO ₄	4.0	26	<i>man-9</i>	264.3	<i>mic-9</i>	260.0
		CuSO ₄	4.6		<i>man-10</i>	52.9	<i>mic-10</i>	73.4
		CuSO ₄	5.6		<i>man-11</i>	67.8	<i>mic-11</i>	50.4
III	Incubation temperature	CaCl ₂	4.0	24	<i>man-12</i>	262.0	<i>mic-12</i>	183.0
		CaCl ₂		28	<i>man-13</i>	44.0	<i>mic-13</i>	306.0
		CaCl ₂		30	<i>man-14</i>	528.0	<i>mic-14</i>	148.0
		CuSO ₄		24	<i>man-15</i>	62.0	<i>mic-15</i>	1194.0
		CuSO ₄	4.0	28	<i>man-16</i>	278.0	<i>mic-16</i>	1012.0
		CuSO ₄		30	<i>man-17</i>	448.0	<i>mic-17</i>	249.0

* pH of the commercial Malt Extract Agar culture media

Table S2. Molecular ions and formulas of compounds isolated from the genus *Pestalotiopsis*

Compound	Formula	Molecular ion <i>m/z</i>	Source	Reference
Ficifuranone B	C ₈ H ₁₀ O ₄	171.0655 [M + H] ⁺	<i>P. fici</i>	[1]
Ficifuranone A	C ₉ H ₁₂ O ₄	185.0811 [M + H] ⁺	<i>P. fici</i>	[1]
4-(2, 4, 7-trioxa-bicyclo[4.1.0]heptan-e-yl)phenol	C ₁₀ H ₁₁ O ₄	195.0657 [M + H] ⁺	<i>P. mangiferae</i>	[2]
Pestaolide	C ₁₂ H ₂₀ O ₂	196.1463 [M] ⁺	<i>P. sp.</i> PSU-MA69	[3]
Pestalotiopyrone N	C ₁₀ H ₂₉ O ₅	209.0455 [M - H] ⁻	<i>P. neglecta</i> SCSI41403	[4]
6-[(7S, 8R)-8-propyloxiran-1-yl]-4-methoxy-pyran-2-one	C ₁₁ H ₁₅ O ₄	211.0965 [M + H] ⁺	<i>P. versicolor</i>	[5]
Pestatheranone A	C ₁₂ H ₁₉ O ₃	211.1329 [M + H] ⁺	<i>P. theaea</i>	[6]
Pestalofuranone A	C ₁₁ H ₁₄ O ₃ Na	217.0835 [M + Na] ⁺	<i>P. besseyi</i>	[7]
Pestalofuranone B	C ₁₁ H ₁₄ O ₃ Na	217.0835 [M + Na] ⁺	<i>P. besseyi</i>	[7]
Pestalofuranone D	C ₁₁ H ₁₄ O ₃ Na	217.0835 [M + Na] ⁺	<i>P. besseyi</i>	[7]
Pestalactam E	C ₁₀ H ₁₃ NO ₃ Na	218.0788 [M + Na] ⁺	<i>P. sp.</i>	[8]
Pestalofuranone C	C ₁₁ H ₁₆ O ₃ Na	219.0992 [M + Na] ⁺	<i>P. besseyi</i>	[7]
Pestalofuranone E	C ₁₁ H ₁₆ O ₃ Na	219.0992 [M + Na] ⁺	<i>P. besseyi</i>	[7]
4, 6-dihydroxy-7-formyl-3-methylcoumarin	C ₁₁ H ₉ O ₅	221.0444 [M + H] ⁺	<i>P. versicolor</i>	[5]
Pestalochromone C	C ₁₁ H ₁₁ ClO ₃	226.0391 [M] ⁺	<i>P. sp.</i> PSU-MA69	[3]
Microsporaline C	C ₁₂ H ₁₄ O ₃ Na	229.0835 [M + Na] ⁺	<i>P. microspora</i> SC3082	[9]
Heterocornol C	C ₁₂ H ₁₄ O ₃ Na	229.0841 [M + Na] ⁺	<i>P. heterocornis</i>	[10]
Pestaloficiol S	C ₁₅ H ₁₇ O ₂	229.1223 [M + H] ⁺	<i>P. fici</i>	[11]
Pestalactam D	C ₁₀ H ₁₃ ³⁵ ClNO ₃	230.0584 [M + H] ⁺	<i>P. sp.</i>	[8]
Pestalotioquinol C	C ₁₃ H ₁₁ O ₄	231.0663 [M - H] ⁻	<i>P. neglecta</i>	[12]
Pestalotioquinol D	C ₁₃ H ₁₁ O ₄	231.0663 [M - H] ⁻	<i>P. neglecta</i>	[12]
Pestalrone A	C ₁₁ H ₁₉ O ₅ ; C ₁₁ H ₁₈ O ₅ Na	231.1227 [M + H] ⁺ ; 253.1046 [M + Na] ⁺	<i>P. zonata</i>	[13]
Pestallic acid G	C ₁₃ H ₁₄ NO ₃	232.0968 [M + H] ⁺	<i>P. neglecta</i> SCSI41403	[4]
Isopolisin B	C ₁₂ H ₁₈ O ₃ Na	233.1154 [M + Na] ⁺	<i>P. heterocornis</i>	[14]
Pestalpyrone D	C ₁₂ H ₁₃ O ₅	237.0757 [M + H] ⁺	<i>P. sp.</i>	[15]
Pestalpyrone E	C ₁₂ H ₁₃ O ₅	237.0757 [M + H] ⁺	<i>P. sp.</i>	[15]
Pestaloisocoumarin A	C ₁₂ H ₁₃ O ₅	237.0763 [M - H] ⁻	<i>P. heterocornis</i>	[14]
Pestalrone B	C ₁₁ H ₁₈ O ₄ Na	237.1088 [M + Na] ⁺	<i>P. karstenii</i>	[16]
Foedanolide	C ₁₄ H ₂₁ O ₃	237.1485 [M + H] ⁺	<i>P. foedan</i>	[17]

Pestalotiol A	C ₁₁ H ₂₀ O ₄ Na	239.1259 [M + Na] ⁺	<i>P. heterocornis</i>	[14]
Heterocornol D	C ₁₂ H ₁₂ O ₄ Na	243.0633 [M + Na] ⁺	<i>P. heterocornis</i>	[10]
Pestalotiopamide E	C ₁₁ H ₁₈ NO ₅	244.1185 [M + H] ⁺	<i>P. sp.</i>	[18]
Vaccinol N	C ₁₂ H ₁₄ O ₄ Na	245.0784 [M + Na] ⁺	<i>P. vaccinii</i>	[19]
Pestalotiopisorin B	C ₁₂ H ₁₄ O ₄ Na	245.0790 [M + Na] ⁺	<i>P. sp</i> HHL101	[20]
Vaccinol L	C ₁₂ H ₁₆ O ₄ Na	247.0941 [M + Na] ⁺	<i>P. vaccinii</i>	[19]
Heterocornol A	C ₁₂ H ₁₆ O ₄ Na	247.0946 [M + Na] ⁺	<i>P. heterocornis</i>	[10]
4, 10-dihydroxy-gamahorin	C ₁₂ H ₁₄ O ₆ Na	249.1097 [M + Na] ⁺	<i>P. sp.</i> M-23	[21]
Vaccinol M	C ₁₂ H ₁₈ O ₄ Na	249.1097 [M + Na] ⁺	<i>P. vaccinii</i>	[19]
Pestaloficiol R	C ₁₃ H ₁₅ O ₅	251.0914 [M + H] ⁺	<i>P. fici</i>	[11]
Disseminin D (9, 10-cis)	C ₁₃ H ₂₄ O ₅ Na	251.1623 [M + Na] ⁺	<i>P. disseminata</i>	[22]
Disseminin E (9, 10-trans)	C ₁₃ H ₂₄ O ₅ Na	251.1623 [M + Na] ⁺	<i>P. disseminata</i>	[22]
Pestaisocoumarin A	C ₁₂ H ₁₂ O ₆	253.0706 [M + H] ⁺	<i>P. heterocornis</i>	[23]
Photopyrone B	C ₁₁ H ₁₈ O ₅ Na	253.1040 [M + Na] ⁺	<i>P. photiniae</i>	[24]
Photopyrone C	C ₁₁ H ₁₈ O ₅ Na	253.1043 [M + Na] ⁺	<i>P. photiniae</i>	[24]
Pestalotioprolide G	C ₁₄ H ₂₁ O ₄	253.1434 [M + H] ⁺	<i>P. microspora</i>	[25]
Spiciferone D	C ₁₄ H ₂₃ O ₄	255.1596 [M + H] ⁺	<i>P. disseminata</i>	[22]
Spiciferone E	C ₁₄ H ₂₃ O ₄	255.1596 [M + H] ⁺	<i>P. disseminata</i>	[22]
Pestalol D	C ₁₄ H ₁₈ O ₃ Na	257.1153 [M + Na] ⁺	<i>P. sp.</i> AcBC2	[26]
Pestalotioprolide C	C ₁₄ H ₂₅ O ₄	257.1747 [M + H] ⁺	<i>P. microspora</i>	[25]
Microsporaline A	C ₁₂ H ₁₄ O ₅ Na	261.0733 [M + Na] ⁺	<i>P. microspora</i> SC3082	[9]
Microsporaline B	C ₁₂ H ₁₆ O ₅ Na	263.0890 [M + Na] ⁺	<i>P. microspora</i> SC3082	[9]
Pestallic acid F	C ₁₄ H ₁₅ O ₅	263.0925 [M - H] ⁻	<i>P. neglecta</i> SCSI41403	[4]
Pestalactam F	C ₁₁ H ₁₅ NO ₅ Na	264.0842 [M + Na] ⁺	<i>P. sp.</i>	[8]
Pestalotiorin	C ₁₄ H ₁₆ O ₅	264.0992 [M] ⁺	<i>P. sp.</i> PSU-ES194	[27]
Pestalactone C	C ₁₃ H ₁₃ O ₆	265.0707 [M + H] ⁺	<i>P. sp.</i>	[15]
Disseminin A	C ₁₃ H ₂₂ O ₄ Na	265.1416 [M + Na] ⁺	<i>P. disseminata</i>	[22]
Disseminin B	C ₁₃ H ₂₂ O ₄ Na	265.1416 [M + Na] ⁺	<i>P. disseminata</i>	[22]
Ficipyrone B	C ₁₄ H ₁₈ O ₅	267.1224 [M + H] ⁺	<i>P. fici</i>	[1]
Disseminin C	C ₁₃ H ₂₄ O ₄ Na	267.1572 [M + Na] ⁺	<i>P. disseminata</i>	[22]
Pestalotioprolide H	C ₁₅ H ₂₃ O ₄	267.1591 [M + H] ⁺	<i>P. microspora</i>	[25]
2-hydroxy-7, 8-epoxy-isodrimeninol	C ₁₅ H ₂₄ O	268.1675 [M] ⁺	<i>P. sp.</i> M-23	[21]
Pestalotioprolide E	C ₁₄ H ₂₄ O ₄ N	270.1700 [M + NH ₄] ⁺	<i>P. microspora</i>	[25]
Pestalotioprolide F	C ₁₄ H ₂₄ O ₄ N	270.1700 [M + NH ₄] ⁺	<i>P. microspora</i>	[25]

Heterocornol M	C ₁₅ H ₂₀ O ₃ Na	271.1310 [M + Na] ⁺	<i>P. heterocornis</i> XWS03F09	[28]
Ficipyrone A	C ₁₄ H ₂₂ O ₅	271.1535 [M + H] ⁺	<i>P. fici</i>	[1]
Pestalotionol	C ₁₄ H ₁₈ O ₃ K	273.0893 [M + K] ⁺	<i>P. sp.</i> PSU-ES194	[27]
Vaccinol K	C ₁₄ H ₁₈ O ₄ Na	273.1097 [M + Na] ⁺	<i>P. vaccinii</i>	[19]
Heterocornol B	C ₁₄ H ₁₈ O ₄ Na	273.1103 [M + Na] ⁺	<i>P. heterocornis</i>	[10]
Heterocornol N	C ₁₄ H ₁₈ O ₄ Na	273.1103 [M + Na] ⁺	<i>P. heterocornis</i> XWS03F09	[28]
11-dehydro-3-hydroxyisodrimeninol	C ₁₅ H ₂₂ O ₃ Na	273.1461 [M + Na] ⁺	<i>P. sp.</i> M-23	[21]
Heterocornol G	C ₁₇ H ₂₁ O ₃	273.1491 [M - H] ⁻	<i>P. heterocornis</i>	[10]
Pestalochromone A	C ₁₂ H ₁₇ ClO ₅	276.0759 [M] ⁺	<i>P. sp.</i> PSU-MA69	[3]
Pestalochromone B	C ₁₂ H ₁₇ ClO ₅	276.0759 [M] ⁺	<i>P. sp.</i> PSU-MA69	[3]
Neopestalone	C ₁₄ H ₁₃ O ₆	277.0707 [M + H] ⁺	<i>P. neglecta</i> SCSI41403	[4]
Pestaloisocoumarin B	C ₁₄ H ₁₅ O ₆	279.0869 [M - H] ⁻	<i>P. heterocornis</i>	[14]
Pestalactone A	C ₁₄ H ₁₇ O ₆	281.1020 [M + Na] ⁺	<i>P. sp.</i>	[15]
Heterocornol O	C ₁₅ H ₁₈ O ₄ Na	285.1103 [M + Na] ⁺	<i>P. heterocornis</i> XWS03F09	[28]
Heterocornol P	C ₁₅ H ₁₈ O ₄ Na	285.1103 [M + Na] ⁺	<i>P. heterocornis</i> XWS03F09	[28]
Microsporaline D	C ₁₄ H ₁₆ O ₅ Na	287.0890 [M + Na] ⁺	<i>P. microspora</i> SC3082	[9]
7--methylNigrosporolide	C ₁₅ H ₂₂ O ₄ Na	289.1410 [M + Na] ⁺	<i>P. microspora</i>	[25]
Pestalotioprolide D	C ₁₅ H ₂₂ O ₄ Na	289.1410 [M + Na] ⁺	<i>P. microspora</i>	[25]
Pestalotioprolide B	C ₁₄ H ₂₀ O ₅ Na	291.1203 [M + Na] ⁺	<i>P. microspora</i>	[25]
2,8-dihydroxy-6,7-en-isodrimeninol	C ₁₅ H ₂₄ O ₄ Na	291.1567 [M + Na] ⁺	<i>P. sp.</i> M-23	[21]
Pestaloporonin B	C ₁₅ H ₂₄ O ₄ Na	291.1572 [M + Na] ⁺	<i>P. sp.</i>	[29]
Heterocornol I	C ₁₇ H ₂₃ O ₄	291.1596 [M - H] ⁻	<i>P. heterocornis</i>	[10]
Heterocornol J	C ₁₇ H ₂₃ O ₄	291.1596 [M - H] ⁻	<i>P. heterocornis</i>	[10]
Heterocornol K	C ₁₇ H ₂₃ O ₄	291.1596 [M - H] ⁻	<i>P. heterocornis</i>	[10]
Vaccinol J	C ₁₇ H ₂₀ O ₃ Na	295.1305 [M + Na] ⁺	<i>P. vaccinii</i>	[19]
Pestaloporonin A	C ₁₆ H ₂₃ O ₅	295.1545 [M - H] ⁻	<i>P. sp.</i>	[29]
Heterocornol H	C ₁₇ H ₂₄ O ₃ Na	299.1623 [M + Na] ⁺	<i>P. heterocornis</i>	[10]
Pestalol E	C ₁₃ H ₁₇ O ₆ S	301.0745 [M + H] ⁺	<i>P. sp.</i> AcBC2	[26]
Pestauvicolactone A	C ₁₆ H ₁₆ NO ₅	302.1023 [M + H] ⁺	<i>P. uvicola</i>	[30]
Pestalactone B	C ₁₃ H ₁₄ O ₇ Na	305.0632 [M + Na] ⁺	<i>P. sp.</i>	[15]
Vaccinol R	C ₁₇ H ₂₃ O ₅	307.1540 [M + H] ⁺	<i>P. vaccinii</i>	[19]

Vaccinol S	C ₁₇ H ₂₃ O ₅	307.1540 [M + H] ⁺	<i>P. vaccinii</i>	[19]
Pestalotioquinol E	C ₂₁ H ₂₅ O ₂	309.1860 [M - H] ⁻	<i>P. neglecta</i>	[12]
Pestalol A	C ₁₉ H ₂₈ O ₂ Na	311.1987 [M + Na] ⁺	<i>P. sp. AcBC2</i>	[26]
Vaccinol O	C ₁₇ H ₂₂ O ₄ Na	313.1410 [M + Na] ⁺	<i>P. vaccinii</i>	[19]
Heterocornol F	C ₁₇ H ₂₄ O ₄ Na	315.1572 [M + Na] ⁺	<i>P. heterocornis</i>	[10]
Pestalol B	C ₁₉ H ₂₆ O ₃ Na	325.1779 [M + Na] ⁺	<i>P. sp. AcBC2</i>	[26]
Pestaloxanthone	C ₁₇ H ₁₄ O ₇	330.0734 [M] ⁺	<i>P. sp. PSU-MA69</i>	[3]
Vaccinol P	C ₁₇ H ₂₄ O ₅ Na	331.1516 [M + Na] ⁺	<i>P. vaccinii</i>	[19]
14-acetylhumulane	C ₁₇ H ₂₄ O ₅ Na	331.1516 [M + Na] ⁺	<i>P. sp.</i>	[31]
Pestaloporinate F	C ₁₇ H ₂₆ O ₅ Na	333.1672 [M + Na] ⁺	<i>P. sp.</i>	[31]
(10S)-12, 16-epoxy-17(15→16)-abeo-3, 5, 8, 12, 15-abietapentaen-2, 7, 11, 14-tetraone	C ₂₀ H ₁₅ O ₅ ⁻	335.0919 [M - H] ⁻	<i>P. adusta</i>	[32]
Pestalotic acid D	C ₁₈ H ₂₃ ClO ₄	338.1285 [M] ⁺	<i>P. sp. cr014</i>	[33]
Pestaloficiol Q	C ₁₈ H ₂₄ O ₅ Na	343.1516 [M + Na] ⁺	<i>P. fici</i>	[11]
Pestalol C	C ₁₉ H ₂₈ O ₄ Na	343.1885 [M + Na] ⁺	<i>P. sp. AcBC2</i>	[26]
Pestalotioquinol B	C ₂₁ H ₂₇ O ₄	343.1909 [M - H] ⁻	<i>P. microspora</i>	[34]
Pestalotione A	C ₁₇ H ₁₃ O ₈	345.0605 [M + H] ⁺	<i>P. theae</i>	[35]
Pestalotic acid B	C ₁₉ H ₂₁ O ₆	345.1338 [M - H] ⁻	<i>P. sp. cr014</i>	[33]
Pestalic acid B	C ₁₈ H ₂₆ O ₅ Na	345.1672 [M + Na] ⁺	<i>P. sp. FT172</i>	[36]
Pestalic acid D	C ₁₈ H ₂₆ O ₅ Na	345.1672 [M + Na] ⁺	<i>P. sp. FT172</i>	[36]
Pestaloporinate C	C ₁₈ H ₂₆ O ₅ Na	345.1672 [M + Na] ⁺	<i>P. sp.</i>	[31]
Pestaloporinate D	C ₁₈ H ₂₆ O ₅ Na	345.1672 [M + Na] ⁺	<i>P. sp.</i>	[31]
Dechloromaldoxin	C ₁₇ H ₁₅ O ₈	347.0761 [M + H] ⁺	<i>P. fici</i>	[37]
Pestaloporinate G	C ₁₈ H ₂₈ O ₅ Na	347.1829 [M + Na] ⁺	<i>P. sp.</i>	[31]
Pestalotic acid A	C ₁₉ H ₂₅ O ₆	349.1651 [M - H] ⁻	<i>P. sp. cr014</i>	[33]
Pestalotione B	C ₁₉ H ₁₉ O ₇	359.1125 [M + H] ⁺	<i>P. theae</i>	[35]
Pestaloporinate B	C ₁₈ H ₂₄ O ₆ Na	359.1465 [M + Na] ⁺	<i>P. sp.</i>	[31]
Pestaloether B	C ₁₆ H ₁₅ ClO ₆ Na	361.0455 [M + Na] ⁺	<i>P. sp. PSU-MA69</i>	[3]
Pestalic acid C	C ₁₈ H ₂₆ O ₆ Na	361.1622 [M + Na] ⁺	<i>P. sp. FT172</i>	[36]
Cytosporin M	C ₁₉ H ₃₀ O ₅ Na	361.1970 [M + Na] ⁺	<i>P. sp. IQ-011</i>	[38]
2'-aminodechloromaldoxin	C ₁₇ H ₁₆ NO ₈	362.0876 [M + H] ⁺	<i>P. flavidula</i>	[39]
2'-aminodechlorogeododoxin	C ₁₇ H ₁₆ NO ₈	362.0876 [M + H] ⁺	<i>P. flavidula</i>	[39]
Pestaloether D	C ₁₈ H ₁₈ O ₈	362.0996 [M] ⁺	<i>P. sp. PSU-MA69</i>	[3]
Vaccinol Q	C ₁₂ H ₁₁ O ₃ Na	363.1778 [M + Na] ⁺	<i>P. vaccinii</i>	[19]
Pestalotioquinol A	C ₂₁ H ₂₈ O ₄ Na	367.1885 [M + Na] ⁺	<i>P. microspora</i>	[34]

Sinopestalotiolide A	C ₂₁ H ₂₁ O ₆	369.1333 [M - H] ⁻	<i>P. palmarum</i>	[40]
Sinopestalotiolide B	C ₂₁ H ₂₁ O ₆	369.1333 [M - H] ⁻	<i>P. palmarum</i>	[40]
Pestynol	C ₂₁ H ₃₀ O ₆ Na	369.2042 [M + Na] ⁺	<i>P. humus</i>	[41]
Ambuic acid derivative 4	C ₁₉ H ₂₄ O ₆ Na	371.1463 [M + Na] ⁺	<i>P. sp.</i>	[42]
Pestalotic acid F	C ₁₉ H ₂₄ O ₆ Na	371.1471 [M + Na] ⁺	<i>P. sp. cr014</i>	[33]
Heterocornol L	C ₁₉ H ₂₄ O ₆ Na	371.1471 [M + Na] ⁺	<i>P. heterocornis</i>	[10]
Sinopestalotiolide C	C ₂₁ H ₂₃ O ₆	371.1489 [M - H] ⁻	<i>P. palmarum</i>	[40]
Pestathenol A	C ₁₉ H ₂₈ O ₆ Na	375.1778 [M + Na] ⁺	<i>P. theae</i>	[6]
Pestathenol B	C ₁₉ H ₂₈ O ₆ Na	375.1778 [M + Na] ⁺	<i>P. theae</i>	[6]
Ambuic acid derivative 3	C ₁₉ H ₂₈ O ₆ Na	375.1778 [M + Na] ⁺	<i>P. sp.</i>	[42]
Ambuic acid derivative 5	C ₁₉ H ₂₈ O ₆ Na	375.1778 [M + Na] ⁺	<i>P. neglecta</i>	[43]
Ambuic acid derivative 6	C ₁₉ H ₂₈ O ₆ Na	375.1778 [M + Na] ⁺	<i>P. sp.</i>	[42]
Pestalotic acid C	C ₁₈ H ₂₅ ClO ₅ Na	379.1288 [M + Na] ⁺	<i>P. sp. cr014</i>	[33]
Pestalic acid E	C ₁₉ H ₂₆ O ₇ Na	385.1571 [M + Na] ⁺	<i>P. sp. FT172</i>	[36]
Ambuic acid derivative 2	C ₁₉ H ₂₄ O ₇ Na	387.14141 [M + Na] ⁺	<i>P. sp.</i>	[42]
Ambuic acid derivative 2	C ₁₉ H ₂₄ O ₇ Na	387.1414 [M + Na] ⁺	<i>P. neglecta</i>	[43]
Virgatolide C	C ₁₉ H ₂₄ O ₇ Na	387.1420 [M + Na] ⁺	<i>P. virgatula</i>	[44]
Virgatolide B	C ₁₉ H ₂₄ O ₇ Na	387.1421 [M + Na] ⁺	<i>P. virgatula</i>	[44]
Pitholide E	C ₂₂ H ₂₇ O ₆	387.1808 [M + H] ⁺	<i>P. microspora</i>	[45]
Pestalotioquinoside C	C ₂₂ H ₂₇ O ₆	387.1813 [M - H] ⁻	<i>P. neglecta</i>	[12]
Ambuic acid derivative 1	C ₁₉ H ₂₆ O ₇ Na	389.1571 [M + Na] ⁺	<i>P. neglecta</i>	[43]
Polyketide-terpene hybrid metabolite 1	C ₁₉ H ₂₆ O ₇ Na	389.1576 [M + Na] ⁺	<i>P. sp.</i>	[46]
Pestalotic acid G	C ₁₉ H ₂₆ O ₇ Na	389.1576 [M + Na] ⁺	<i>P. sp. cr014</i>	[33]
Pestalotic acid H	C ₁₉ H ₂₆ O ₇ Na	389.1576 [M + Na] ⁺	<i>P. sp. cr014</i>	[33]
Pestalotic acid I	C ₁₉ H ₂₆ O ₇ Na	389.1576 [M + Na] ⁺	<i>P. sp. cr014</i>	[33]
Ambuic acid derivative 1	C ₁₉ H ₂₆ O ₇ Na	389.1576 [M + Na] ⁺	<i>P. sp.</i>	[46]
Ambuic acid derivative 5	C ₁₉ H ₂₆ O ₇ Na	389.1576 [M + Na] ⁺	<i>P. sp.</i>	[46]
Polyketide-terpene hybrid metabolite 5	C ₁₉ H ₂₆ O ₇ Na	389.1576 [M + Na] ⁺	<i>P. sp.</i>	[46]
Pestalpolyol E	C ₂₂ H ₃₈ O ₄ Na	389.2668 [M + Na] ⁺	<i>P. sp. PG52</i>	[47]
Pestalone E	C ₂₀ H ₂₀ ³⁵ ClO ₆	391.0948 [M + H] ⁺	<i>P. neglecta</i>	[48]
Pestaloporinate E	C ₂₀ H ₃₂ O ₆ Na	391.2091 [M + Na] ⁺	<i>P. sp.</i>	[31]
Ambuic acid derivative 3	C ₁₉ H ₃₀ O ₇ Na	393.1884 [M + Na] ⁺	<i>P. neglecta</i>	[43]
Pestalotioquinol F	C ₂₂ H ₂₈ O ₅ Na	395.1829 [M + Na] ⁺	<i>P. neglecta</i>	[12]
Pestaloether A	C ₁₈ H ₁₇ ClO ₈	396.0612 [M] ⁺	<i>P. sp. PSU-MA69</i>	[3]
Pestaloether C	C ₁₈ H ₁₇ ClO ₈	396.0612 [M] ⁺	<i>P. sp. PSU-MA69</i>	[3]

Sinopestalotiollide D	C ₂₂ H ₂₃ O ₇	399.1438 [M - H] ⁻	<i>P. palmarum</i>	[40]
Pestalone F	C ₂₁ H ₂₂ ³⁵ ClO ₆	405.1105 [M + H] ⁺	<i>P. neglecta</i>	[48]
Pestaloporinate A	C ₂₀ H ₃₀ O ₇ Na	405.1884 [M + Na] ⁺	<i>P. sp.</i>	[31]
Ambuic acid derivative 5	C ₂₂ H ₃₀ O ₆ Na	413.1935 [M + Na] ⁺	<i>P. sp.</i>	[42]
Pestalotic acid E	C ₂₁ H ₂₆ O ₇ Na	413.2668 [M + Na] ⁺	<i>P. sp. cr014</i>	[33]
Ambuic acid derivative 1	C ₂₁ H ₂₈ O ₇ Na	415.1719 [M + Na] ⁺	<i>P. sp.</i>	[42]
Ambuic acid derivative 4	C ₂₁ H ₃₀ O ₇ Na	417.1884 [M + Na] ⁺	<i>P. neglecta</i>	[43]
Pestazonatic acid	C ₂₀ H ₁₉ O ₁₀	419.0984 [2M - H] ⁻	<i>P. zonata</i>	[13]
(±)-Pestalachloride D	C ₂₁ H ₂₀ Cl ₂ O ₅	422.0682 [M] ⁺	<i>P. sp.</i>	[49]
Pestalpolyol B	C ₂₅ H ₄₂ O ₄ Na	429.2981 [M + Na] ⁺	<i>P. sp. cr013</i>	[50]
Pestalic acid A	C ₂₁ H ₂₈ O ₈ Na	431.1676 [M + Na] ⁺	<i>P. sp. FT172</i>	[36]
Polyketide-terpene hybrid metabolite 2	C ₂₁ H ₂₈ O ₈ Na	431.1682 [M + Na] ⁺	<i>P. sp.</i>	[46]
Polyketide-terpene hybrid metabolite 4	C ₂₁ H ₂₈ O ₈ Na	431.1682 [M + Na] ⁺	<i>P. sp.</i>	[46]
Ambuic acid derivative 2	C ₂₁ H ₂₈ O ₈ Na	431.1682 [M + Na] ⁺	<i>P. sp.</i>	[46]
Ambuic acid derivative 4	C ₂₁ H ₂₈ O ₈ Na	431.1682 [M + Na] ⁺	<i>P. sp.</i>	[46]
Polyketide-terpene hybrid metabolite 3	C ₂₁ H ₃₀ O ₈ Na	433.1838 [M + Na] ⁺	<i>P. sp.</i>	[46]
Ambuic acid derivative 3	C ₂₁ H ₃₀ O ₈ Na	433.1838 [M + Na] ⁺	<i>P. sp.</i>	[46]
Pestalone C	C ₂₀ H ₂₀ ⁷⁹ BrO ₆ C ₂₀ H ₂₀ ⁸¹ BrO ₆	435.0443 [M + H] ⁺ ; 437.0423 [M + H] ⁺	<i>P. neglecta</i>	[48]
Pestalone B	C ₂₁ H ₂₂ ⁷⁹ BrO ₆ C ₂₁ H ₂₂ ⁸¹ BrO ₆	449.0600 [M + H] ⁺ ; 451.0579 [M + H] ⁺	<i>P. neglecta</i>	[48]
Pestalotioquinoside A	C ₂₇ H ₃₅ O ₆	455.2439 [M - H] ⁻	<i>P. neglecta</i>	[12]
Virgatolide A	C ₂₂ H ₂₆ O ₉ Na	457.1466 [M + Na] ⁺	<i>P. virgatula</i>	[44]
Pestalpolyol H	C ₂₈ H ₄₈ O ₄ Na	471.3450 [M + Na] ⁺	<i>P. sp. PG52</i>	[47]
Pestalpolyol A	C ₂₈ H ₅₀ O ₄ Na	473.3607 [M + Na] ⁺	<i>P. sp. cr013</i>	[50]
(±)-Pestaloxazine A	C ₂₂ H ₃₃ N ₄ O ₈	481.22984 [M + H] ⁺	<i>P. sp. ZJ-2009-7-6</i>	[51]
Pestalone G	C ₂₁ H ₂₁ ⁷⁹ Br ³⁵ ClO ₆	483.0210 [M + H] ⁺	<i>P. neglecta</i>	[48]
Pestalone H	C ₂₁ H ₂₁ ⁷⁹ Br ³⁵ ClO ₆	483.0210 [M + H] ⁺	<i>P. neglecta</i>	[48]
Pestaloamide A	C ₂₄ H ₂₄ N ₂ O ₅ S ₂	485.1195 [M + H] ⁺	<i>P. sp. HS30</i>	[52]
Pestalpolyol G	C ₂₈ H ₄₈ O ₅ Na	485.3243 [M + Na] ⁺	<i>P. sp. PG52</i>	[47]
Pestalotione C	C ₂₂ H ₂₄ O ₁₁ Na	487.1216 [M + Na] ⁺	<i>P. theae</i>	[35]
Pestalotioquinoside B	C ₂₇ H ₃₅ O ₈	487.2326 [M + H] ⁺	<i>P. neglecta</i>	[12]
Pestalpolyol F	C ₂₈ H ₄₈ O ₅ Na	487.3399 [M + Na] ⁺	<i>P. sp. PG52</i>	[47]
Pestaloamide B	C ₂₄ H ₂₄ N ₂ O ₅ S ₂	507.1019 [M + Na] ⁺	<i>P. sp. HS30</i>	[52]
11 -acetoxyisoaustinone	C ₂₇ H ₃₂ O ₈ Na	507.1995 [M + Na] ⁺	<i>P. sp. PSU-ES194</i>	[27]

4 ^α , 5 ^β -diacetoxy-9 ^α -benzoyloxy-7 ^α H-eudesman-1 ^α , 2 ^β , 11, 14-tetraol	C ₂₆ H ₃₇ O ₁₀	509.2381 [M + H] ⁺	<i>P.</i> sp.	[53]
7-hydroxydehydroaustin	C ₂₇ H ₃₁ O ₁₀	515.1917 [M + H] ⁺	<i>P.</i> sp. PSU-ES194	[27]
Pestalone D	C ₂₁ H ₂₁ ⁷⁹ BrO ₆	526.9705 [M + H] ⁺	<i>P. neglecta</i>	[48]
Dihydroberkleasmin A	C ₃₀ H ₅₀ O ₇ Na	545.3454 [M + Na] ⁺	<i>P. photiniae</i>	[54]
Pestalotiopen A	C ₂₇ H ₃₃ ClO ₁₀	551.16840 [M - H] ⁻	<i>P.</i> sp.	[55]
Pestalpolyol C	C ₃₃ H ₅₈ O ₅ Na	557.4182 [M + Na] ⁺	<i>P.</i> sp. cr013	[50]
Pestalpolyol D	C ₃₄ H ₆₀ O ₅ Na	571.4338 [M + Na] ⁺	<i>P.</i> sp. cr013	[50]
Pestaloporonin C	C ₃₂ H ₄₈ O ₈ Na	583.3247 [2 M + Na] ⁺	<i>P.</i> sp.	[29]
1 ^β , 5 ^α , 6 ^α , 14-tetraacetoxy-9 ^α -benzoyloxy-7 ^α H-eudesman-2 ^β , 11-diol	C ₃₀ H ₄₁ O ₁₂	593.2593 [M + H] ⁺	<i>P.</i> sp.	[53]
Chloropestolide G	C ₃₂ H ₃₁ ClO ₁₀ Na	633.1498 [M + Na] ⁺	<i>P. fici</i>	[37]
Chloropestolide D	C ₃₃ H ₃₆ ClO ₁₁	643.1941 [M + H] ⁺	<i>P. fici</i>	[37]
Chloropestolide E	C ₃₃ H ₃₆ ClO ₁₁	643.1941 [M + H] ⁺	<i>P. fici</i>	[37]
Chloropupukeanolide E	C ₃₂ H ₃₃ ClO ₁₁ Na	651.1604 [M + Na] ⁺	<i>P. fici</i>	[56]
Chloropestolide B	C ₃₃ H ₃₅ ClO ₁₁ Na	665.1760 [M + Na] ⁺	<i>P. fici</i>	[37]
Chloropestolide C	C ₃₃ H ₃₅ ClO ₁₁ Na	665.1760 [M + Na] ⁺	<i>P. fici</i>	[37]
Chloropestolide F	C ₃₃ H ₃₅ ClO ₁₁ Na	665.1760 [M + Na] ⁺	<i>P. fici</i>	[37]
Chloropupukeanolide C	C ₃₃ H ₃₅ ClO ₁₁ Na	665.1760 [M + Na] ⁺	<i>P. fici</i>	[56]
Chloropupukeanolide D	C ₃₃ H ₃₅ ClO ₁₁ Na	665.1760 [M + Na] ⁺	<i>P. fici</i>	[56]
Pestaloquinol B	C ₃₈ H ₅₂ O ₁₀ Na	691.3453 [M + Na] ⁺	<i>P.</i> sp.	[57]
Pestaloquinol A	C ₃₈ H ₅₂ O ₁₀ Na	691.3453 [M + Na] ⁺	<i>P.</i> sp.	[57]
Torreyanic acid analogue	C ₃₈ H ₄₅ O ₁₂	693.2917 [M - H] ⁻	<i>P.</i> sp.	[42]
Pestalotiopen B	C ₃₄ H ₄₅ ClO ₁₃	695.24704 [M - H] ⁻	<i>P.</i> sp.	[55]
Pestauvicomorpholine A	C ₄₃ H ₅₃ NO ₇ Na	718.3714 [M + Na] ⁺	<i>P. uvicola</i>	[30]
Pestiocandin	C ₄₃ H ₆₂ O ₁₆ Na	857.3936 [M + Na] ⁺	<i>P. humus</i>	[58]
1-undecene-2, 3-dicarboxylic acid	C ₁₃ H ₂₂ O ₄	243.1591	<i>P. theae</i>	[59]
Oxopestalochromane	C ₁₃ H ₁₃ O ₆	265.0710	<i>P.</i> sp. IQ-011	[38]
Chlorotheolide B	C ₂₉ H ₃₂ ClO ₁₀	575.1679	<i>P. theae</i>	[59]
Chlorotheolide A	C ₃₀ H ₃₆ ClO ₁₁	607.1941	<i>P. theae</i>	[59]
Pestalotine D	C ₁₉ H ₂₀ O ₈	Not reported	<i>P. theae</i>	[35]
Cytosporin N	C ₁₉ H ₂₈ O ₆	Not reported	<i>P.</i> sp. IQ-011	[38]
Cuautepestalorin	C ₃₂ H ₃₆ O ₁₀	Not reported	<i>P.</i> sp. IQ-011	[38]
6-(1-hydroxypentyl)-4-methoxy-pyran-2-one		191 [M + Na - CO ₂] ⁺ ; 213 [M + H] ⁺ ;	<i>P. guepinii</i>	[60]

		235 [M + Na] ⁺ ; 447 [2XM + Na] ⁺		
6-hydroxymethyl-4-methoxy-5,6-dihydro-2H-pyran-2-one	C ₇ H ₁₀ O ₄	159.2 [M + H] ⁺	<i>P. sydowiana</i>	[61]
4-(hydroxymethyl)catechol	C ₇ H ₈ O ₃ Na	163.1 [M + Na] ⁺	<i>P. sp.</i>	[62]
(4S)-4, 8-dihydroxy-1-tetralone	C ₁₀ H ₁₀ O ₃	179 [M + H] ⁺	<i>P. sp.</i> EJC07	[63]
Pestalopyrone	C ₁₁ H ₁₂ O ₃	179.1 [M - H] ⁻ ; 181.1 [M + H] ⁺	<i>P. neglecta</i> SCSI41403	[4]
(3R, 4R, 6R, 7S)-7-hydroxyl-3, 7-dimethyl-oxabicyclo[3.3.1]-nonan-2-one	C ₁₀ H ₁₆ O ₃	183 [M - H] ⁻	<i>P. foedan</i>	[64]
2,4-dihydroxy-3,5,6-trimethylbenzoic acid	C ₁₀ H ₁₁ O ₄	195.1 [M - H] ⁻	<i>P. neglecta</i> SCSI41403	[4]
6-pentyl-4-methoxy-pyran-2-one		197 [M + H] ⁺ ; 219 [M + Na] ⁺	<i>P. guepinii</i>	[60]
Pestalotiopyrone G	C ₁₀ H ₁₂ O ₃	202.9 [M + Na] ⁺	<i>P. sydowiana</i>	[61]
Pestalotiopyrone E	C ₁₀ H ₁₄ O ₄	221.0 [M + Na] ⁺	<i>P. sydowiana</i>	[61]
LL-P880b	C ₁₁ H ₁₈ O ₅	231.2 [M + H] ⁺	<i>P. sydowiana</i>	[61]
Pestalotiopyrone D	C ₁₀ H ₁₄ O ₅	237.0 [M + Na] ⁺	<i>P. sydowiana</i>	[61]
Photopyrone	C ₁₁ H ₁₈ O ₅	253.1 [M + Na] ⁺	<i>P. sydowiana</i>	[61]
Sesquicaranoic acid B	C ₁₅ H ₂₃ O ₄	267.3 [M - H] ⁻	<i>P. neglecta</i> SCSI41403	[4]
Citreorosein	C ₁₅ H ₉ O ₆	285.1 [M - H] ⁻	<i>P. neglecta</i> SCSI41403	[4]
Altitoxin B	C ₁₅ H ₂₂ ClO ₄	301 [M - H] ⁻	<i>P. sp.</i>	[55]
dehydroisopenicillide	C ₂₁ H ₂₂ O ₆	371.2 [M + H] ⁺	<i>P. sydowiana</i>	[61]
3'-O-methyldehydroisopenicillide	C ₂₂ H ₂₄ O ₆	385.4 [M + H] ⁺	<i>P. sydowiana</i>	[61]
Pestalotiollide B	C ₂₁ H ₂₂ O ₇	387.4 [M + H] ⁺	<i>P. sydowiana</i>	[61]
Pestalotiollide A	C ₂₁ H ₂₂ O ₇	387.4 [M + H] ⁺	<i>P. sydowiana</i>	[61]
Monocycloalternarene B	C ₂₂ H ₃₁ O ₆	391.2 [M - H] ⁻	<i>P. neglecta</i> SCSI41403	[4]
Pestalone	C ₂₁ H ₂₀ Cl ₂ O ₆	437.1 [M - H] ⁻ ; 439.1 [M + H] ⁺	<i>P. neglecta</i> SCSI41403	[4]