Supplementary Materials

Comparative metabolomics charts distinct chemical repertoires across phytopathogenic fungi

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GNPS JOBS LINKS

Feature-based molecular networking (FBMN) results

Colletotrichum higginsianum

MSDIAL *https://gnps2.org/status?task=258f3792839844d5ba118fac5e95a7a5*

Sclerotinia sclerotiorum

MSDIAL *https://gnps2.org/status?task=ef113642444f4288b2585f732c54a4ec*

Cladosporium cucumerinum

MSDIAL *https://gnps2.org/status?task=e54ba49097374efca3a016c4a7c83b4e*

Phytophthora capsici

MSDIAL *https://gnps2.org/status?task=e10abdcc818f41d2a46b6bed6a97b270*

Phytophthora cinnamomi

MSDIAL *https://gnps2.org/status?task=f96fc44f19394f5fbb49df4a0fac6283*

All-non cereal fungal species

Mzmine*https://gnps2.org/status?task=11abd07ed8944e0f89450b45829edeac*

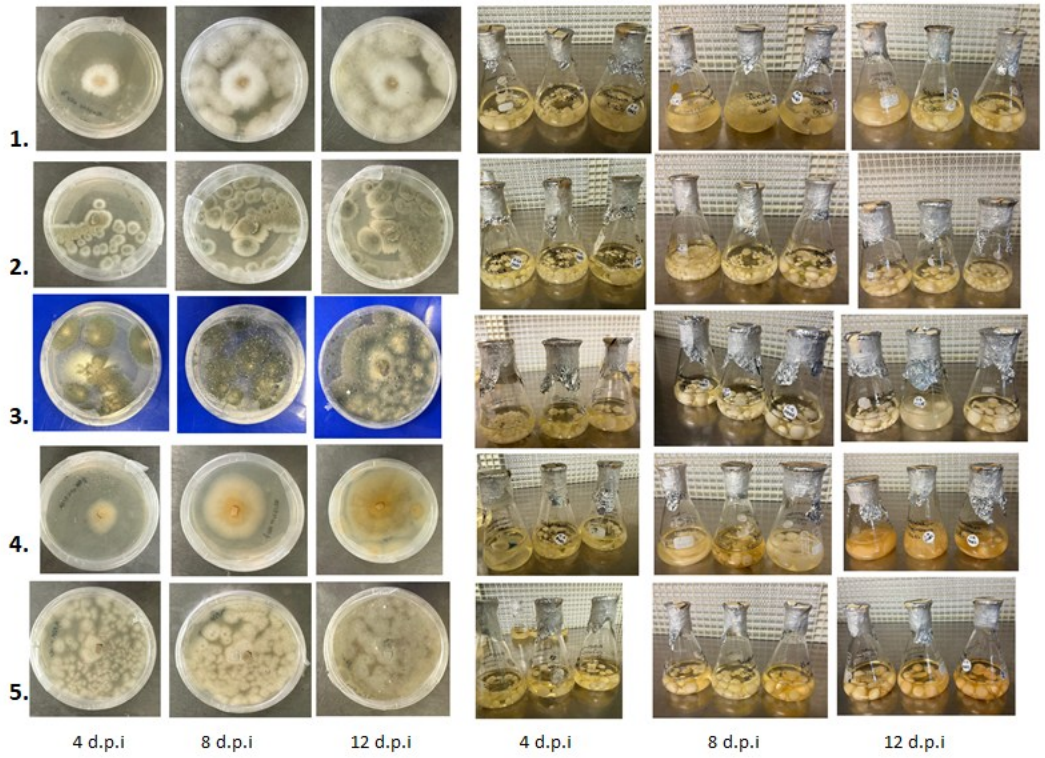

Fig S1: Time-course analysis of fungal growth on both agar plates and liquid media of *Sclerotinia sclerotiorum* (1)*, Phytophthora capsici* (2)*, Cladosporium cucumerinum* (3)*, Colletotrichum higginsianum*(4)*,* and *Phytophthora cinnamomi* (5)*.* Incubation conditions: 25 °C, 12 days, half-strength Potato dextrose agar (19.45 g PDA powder +1L distilled water). Fungal strains were cultured on PDA agar plates and inoculated in liquid potato dextrose broth (PDB) media at 25 °C under sterile conditions shaking at 120 rpm and the biomass was harvested at 4, 8, and 12 day post inoculation (d.p.i) (day 4 showing initial growth and germination, day 8 active growth and hyphae extension, day 12 shows maximum biomass production sporulation).

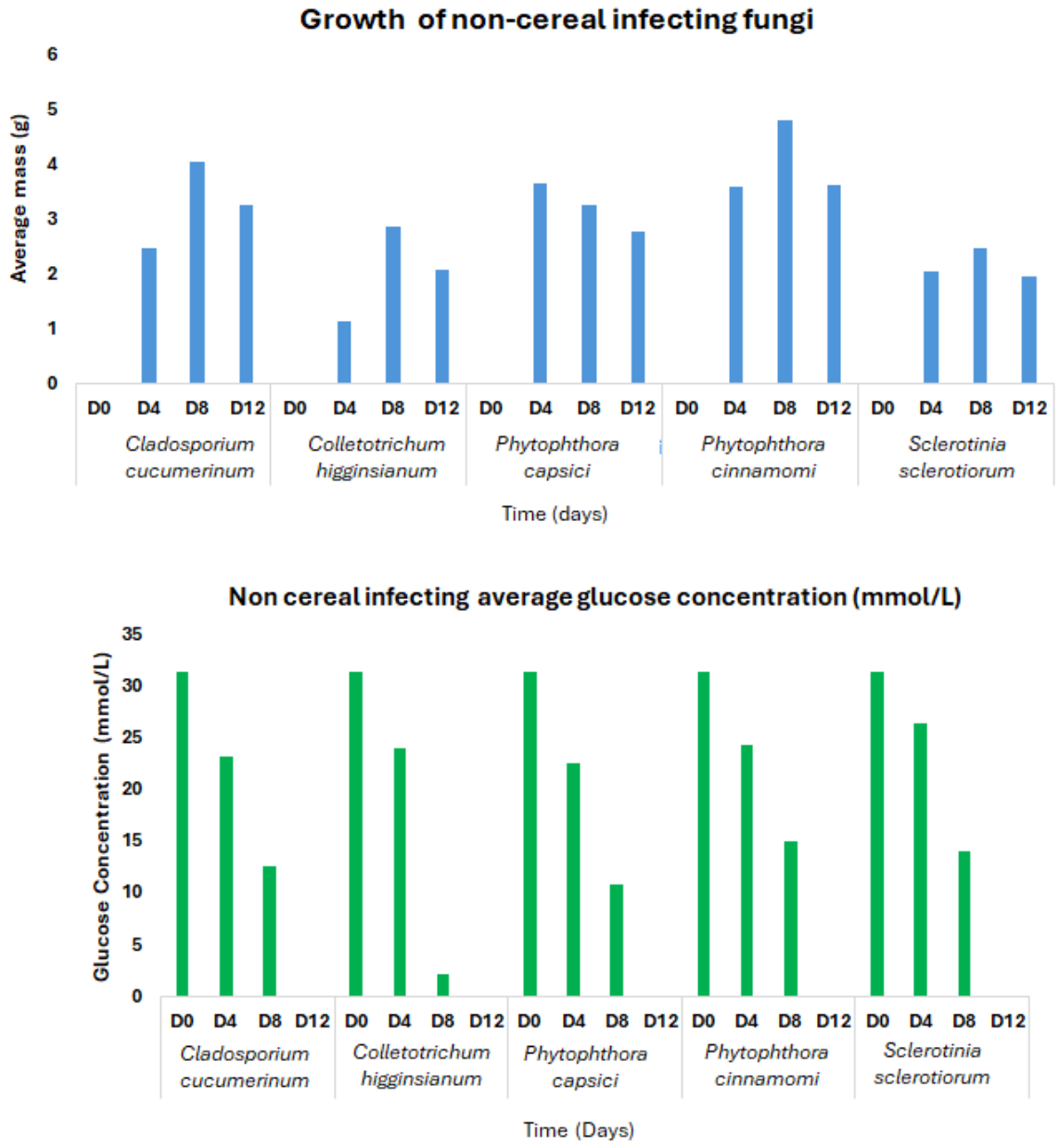

Fig S2: Time-course assessment of glucose consumption and biomass accumulation of non-cereal infecting fungi, *Sclerotinia sclerotiorum, Colletotrichum higginsianum, Phytophthora capsici, Phytophthora cinnamomi,* and *Cladosporium cucumerinum* over time (0, 4, 8 and 12 days). The glucose concentration of the Potato dextrose broth and the biomass of the fungal mycelia of each fungal strain were measured overtime at different time points of harvest.

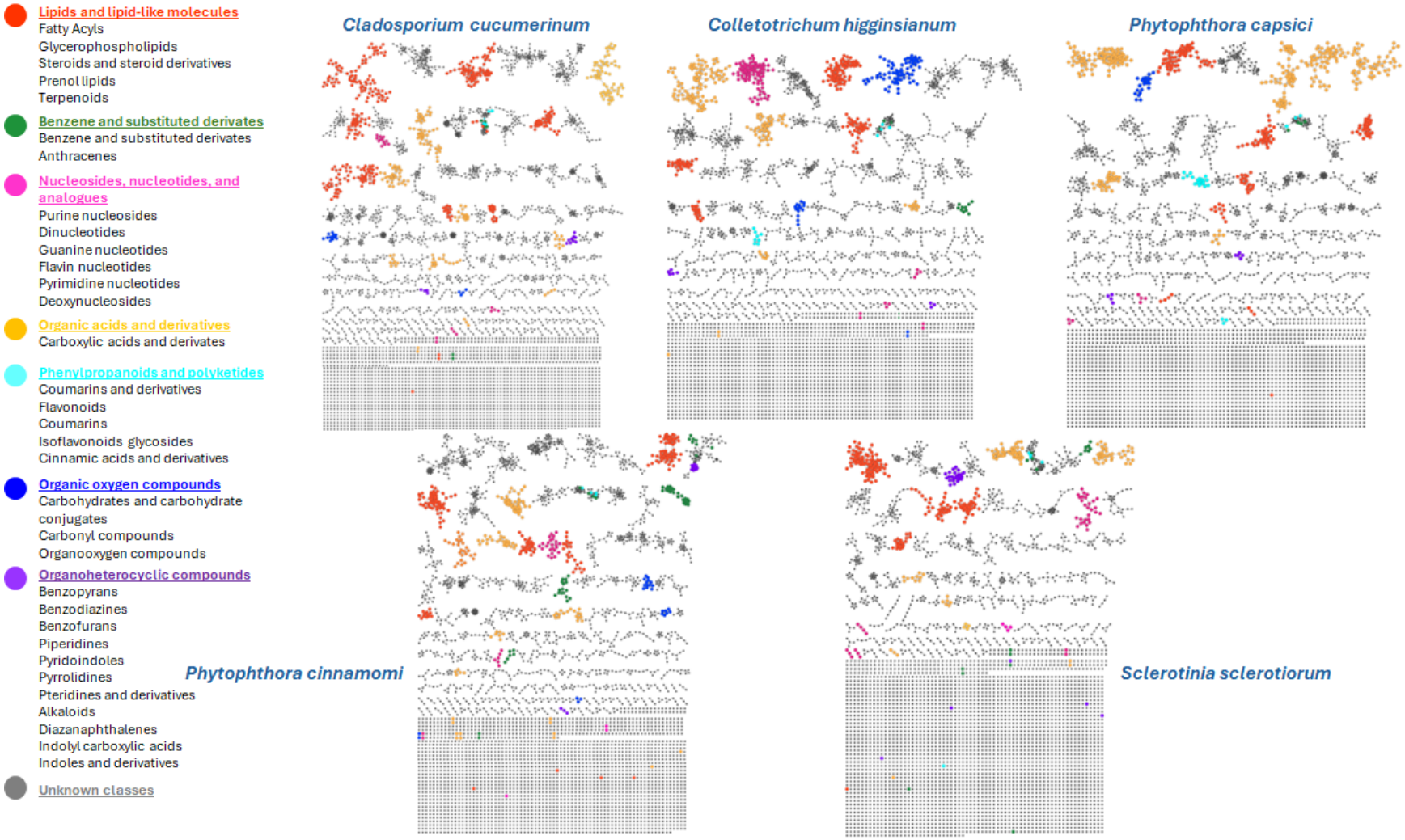

Fig S3: Representation of GNPS mass spectral feature-based networks generated using the ESI negative data from *Sclerotinia sclerotiorum, Phytophthora capsici, Colletotrichum higginsianum, Phytophthora cinnamomi,* and *Cladosporium cucumerinum* metabolite extracts. The networks show a visualization of putatively annotated chemical super-classes (indicated by colored labels corresponding to the node colors) and specific classes (written in black) of non-cereal fungi identified through GNPS library matches.

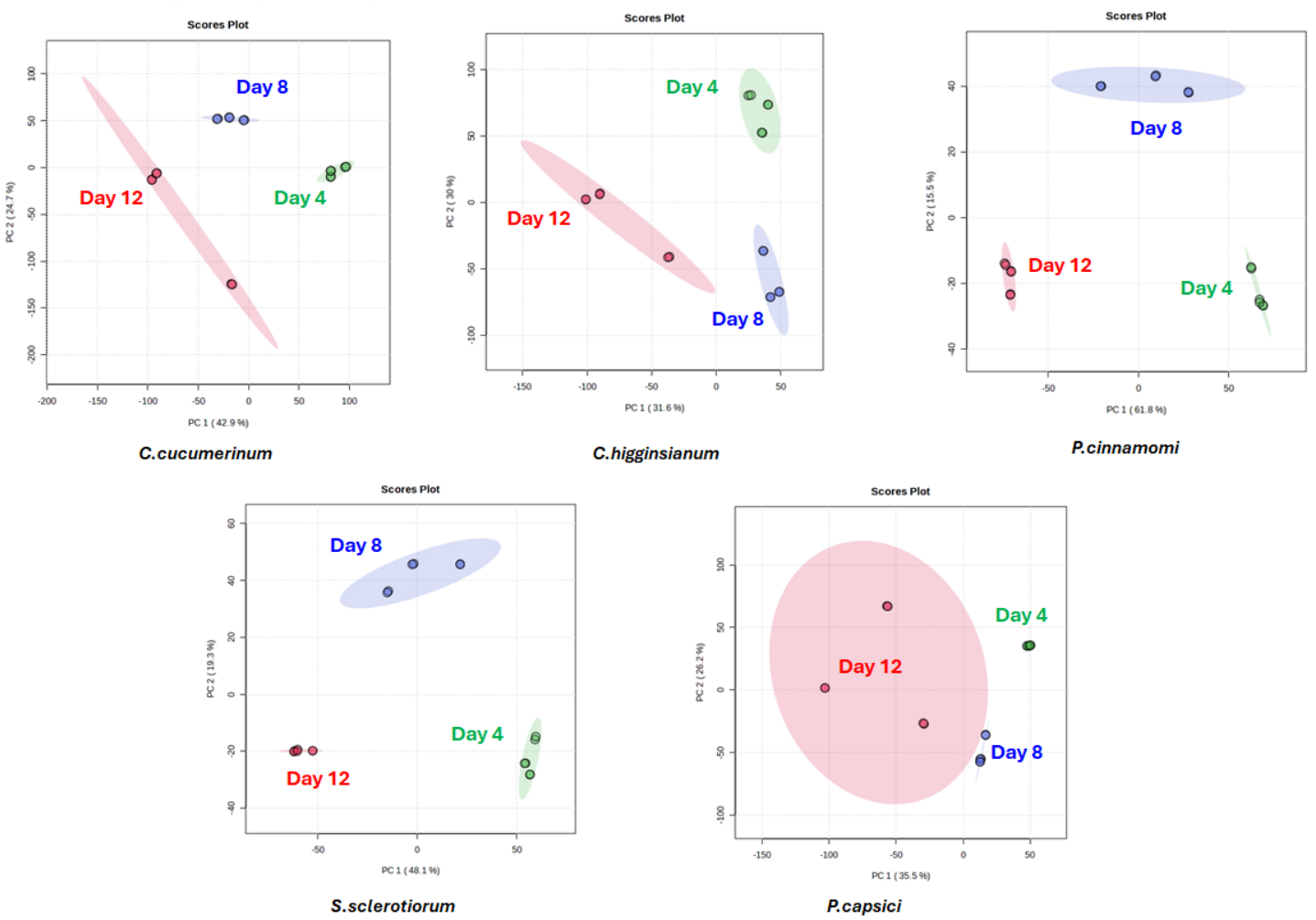

Fig S4: The PCA score plots of the UPLC-MS data of *Sclerotinia sclerotiorum, Phytophthora capsici, Colletotrichum higginsianum, Phytophthora cinnamomi,* and *Cladosporium cucumerinum* metabolite extracts at different time points. PCA scores plots (PC1 vs PC2) of fungal strains cultured and harvested at different growth points: 4, 8, and 12 days post inoculation (d.p.i.). PCA scores plots models with R^2 values greater than 0.60 and *p*-value of 0.001 using Pareto-scaled data showing time-related sample groupings (4, 8, and 12 d.p.i) of all the non-cereal infecting fungal samples.

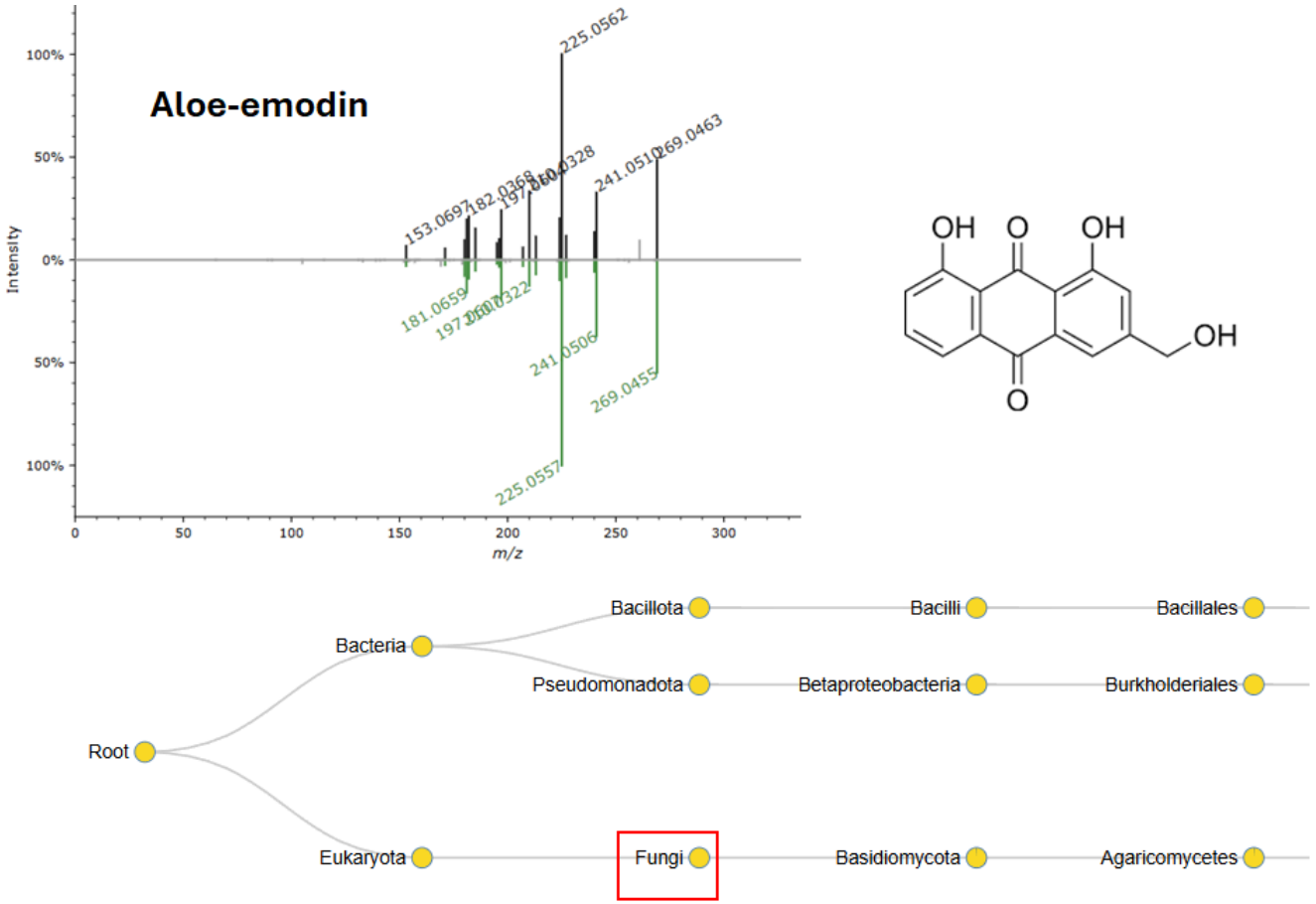

Fig S5: An example of a microbeMASST search of anthraquinones output confirming that eukaryotes such as fungi cultures extracts can produce microbial metabolites, such as Aloe-emodin which were detected from the molecular network of pathogenic fungal isolates (*P.cinnamomi*) generated from the intracellular samples. The pie charts displayed the proportion of MS/MS matches found in the deposited reference database. Blue indicates a match with monocultures, while yellow indicates a non-match.

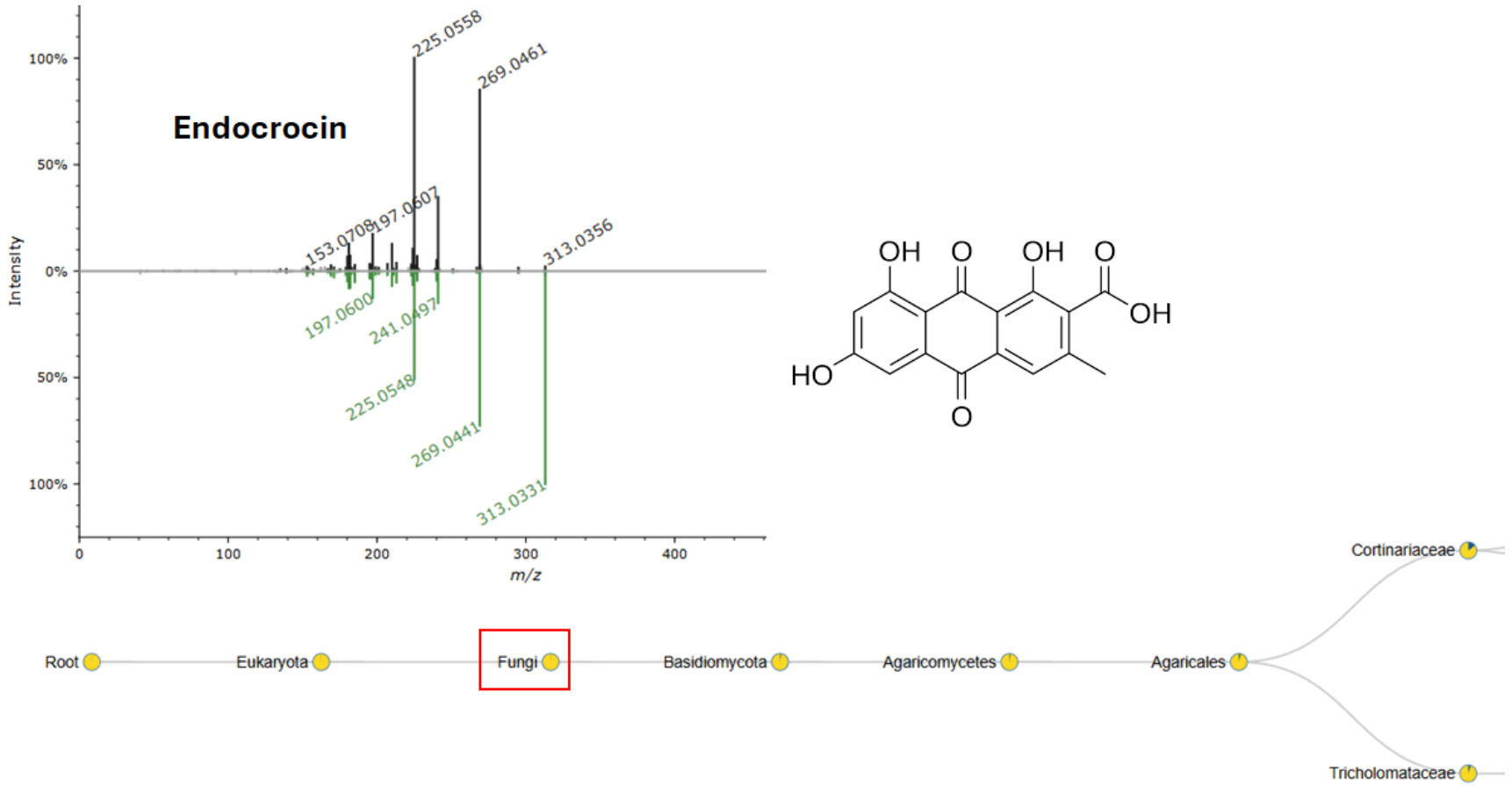

Fig S6: Example output from MicrobeMASST search for polyketides compounds, illustrating eukaryotic organisms such as fungi can produce microbial secondary metabolites. The analysis confirmed the presence of Endocrocin, a known fungal polyketide, within the molecular network generated from intracellular extracts of *Phytophthora cinnamomi* isolates. Accompanying pie charts represent the proportion of MS/MS spectral matches against the curated microbeMASST reference database. Blue segments indicate spectra that matched with known monoculture-derived compounds, while yellow segments represent unmatched spectra, suggesting either novel compounds or compounds not yet present in the reference dataset.

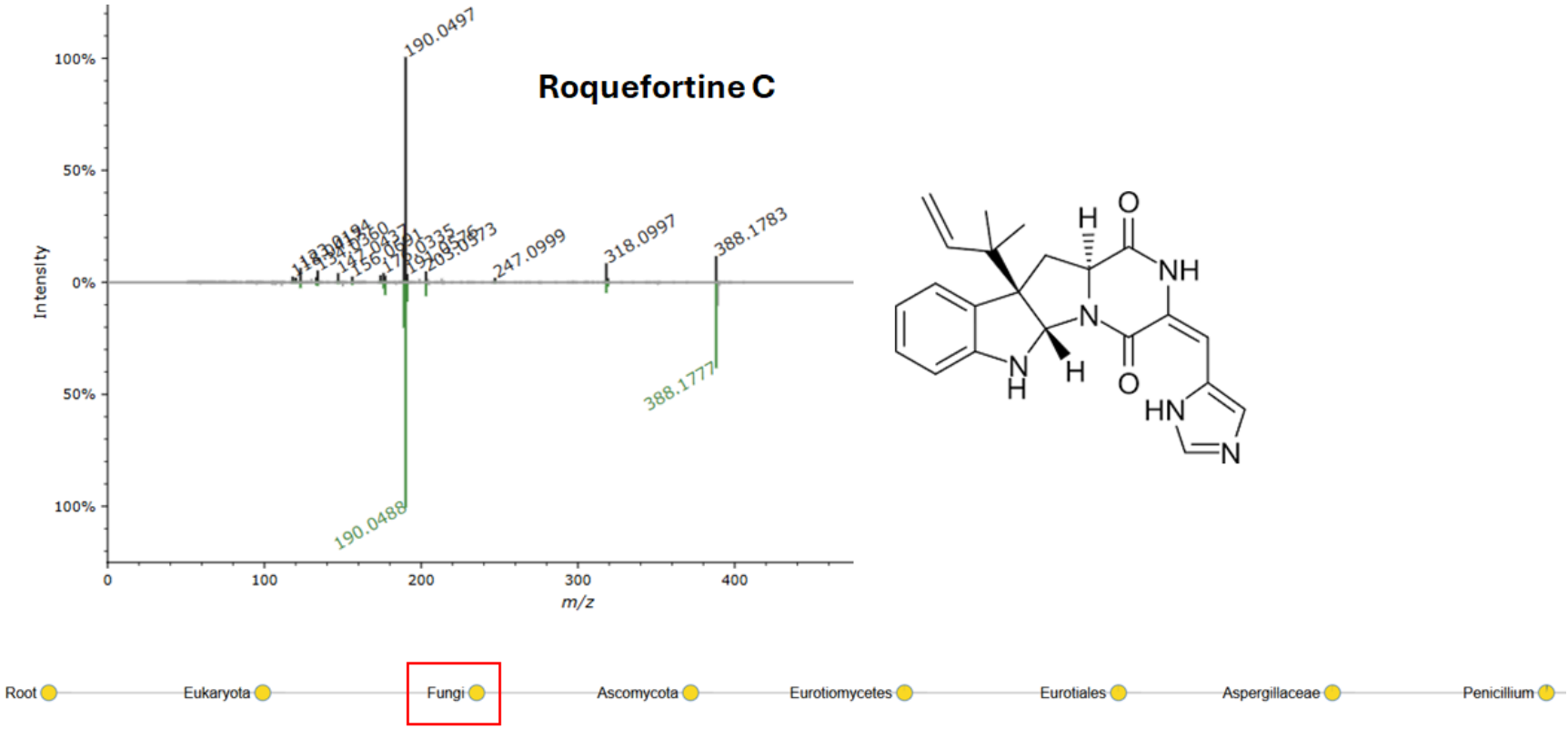

Fig S7: An example of a microbeMASST search of indole alkaloids output confirming that eukaryotes such as fungi cultures extracts can produce microbial metabolites, such as Roquefortine C which were detected from the molecular network of pathogenic fungal isolates generated from the intracellular samples.

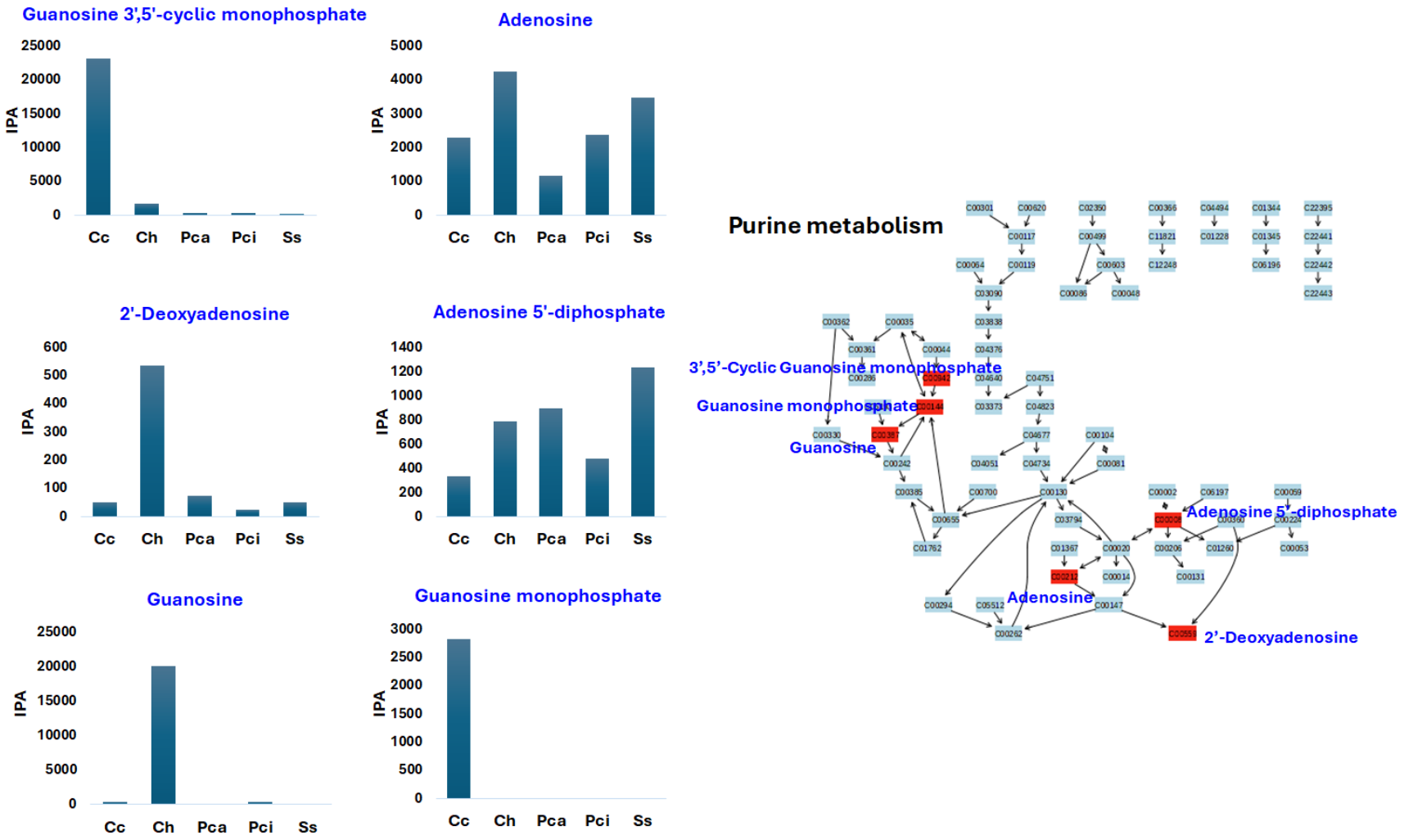

Fig S8: Purines annotated from non-cereal infecting pathogens. Bar graphs display the relative abundance of purine compounds detected in the intracellular extracts from various non-cereal infecting isolates. The accompanying purine metabolism pathway diagram highlights in red the specific purine metabolites that were confidently annotated based on spectral matches. Abbreviations: Cc = *C.cucumerinum*, Ch = *C.higginsianum*, Pca = *P.capsici*, Pci = *P.cinnamomi*, and Ss = *S.sclerotiorum*, IPA = Integrated Peak Area.

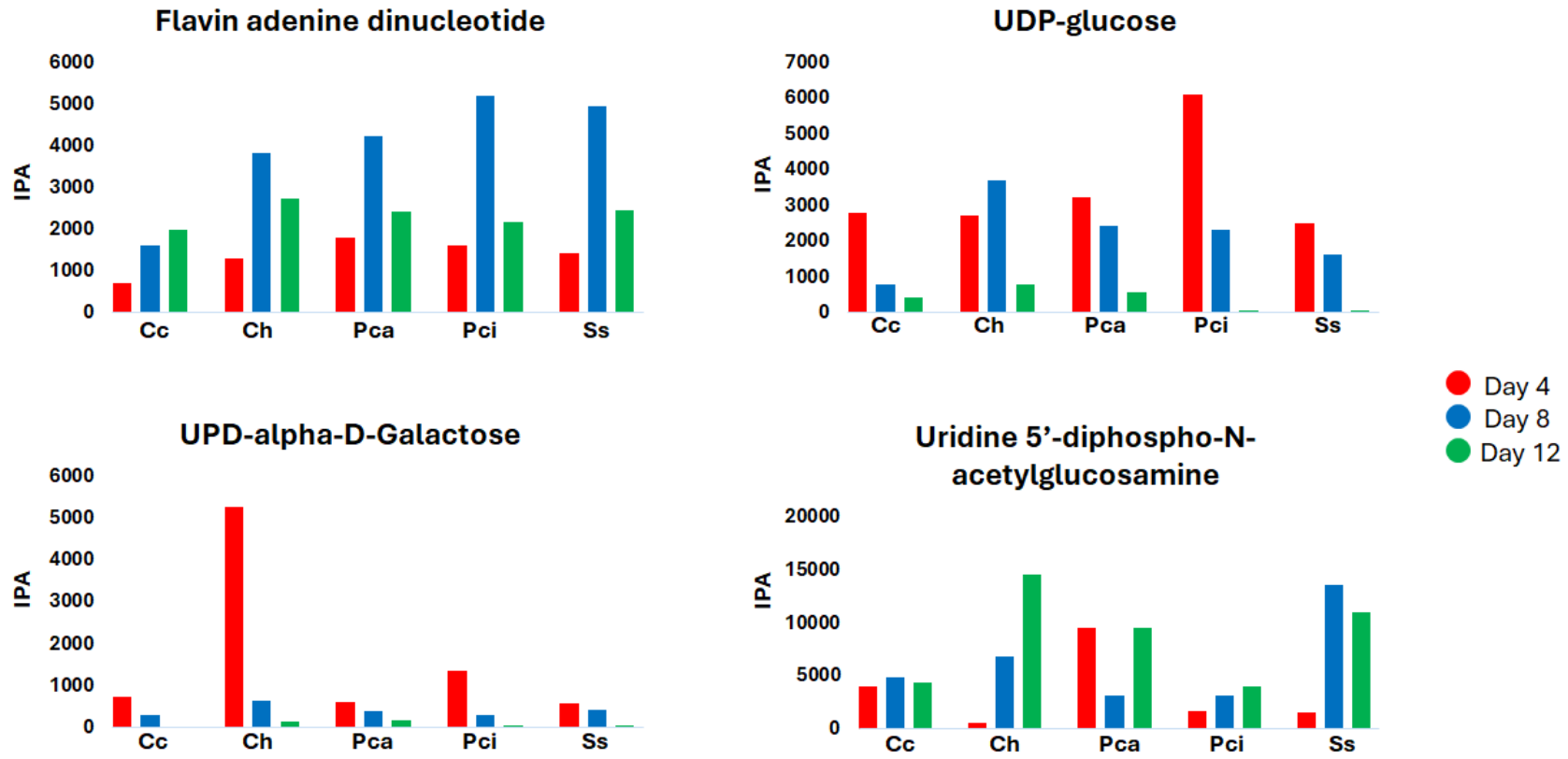

Fig S9: The relative quantification of nucleotides and nucleotide sugars at different growth time points. The bar graphs show levels of annotated nucleotides and nucleotide sugars at different growth phases of the non-cereal infecting fungal cells. Each bar represents the mean intensity area from six replicates (n=6) with calculated *p*-values ≤ 0.05 (showing the significance of the differences between the compared groups). Abbreviations: Cc = *C.cucumerinum*, Ch = *C.higginsianum*, Pca = *P.capsici*, Pci = *P.cinnamomi*, and Ss = *S.sclerotiorum*, IPA = Integrated Peak Area.

Table S1: Metabolite annotation summary. A summary of putative metabolite identifications based on Feature-Based Molecular Networking (FBMN) and GNPS library matches,derived from metabolomics datasets of fungal isolates infecting non-cereal crops and unique metabolites detected in each fungal species (highlighted in blue). This table includes compound names, spectral peaks and associated metadata for each annotation.

Annotated metabolites	Rt (min)	*m/z*	Adducts	Fragmentation ions	Metabolite class	*S. Sclerotiorum*	*P.capsici*	*P.cinnamomi*	*C.cucumerinum*	*C.higginsianum*
LPC 18:1	9.71	566.348	M+HCOO	152.99, 224.0691, 281.24, 506.3267	Glycerophospholipid	✓		✓	✓	✓
LPI 18:0	8.22	599.302	[M-H]-	152.99, 241.01, 283.22, 315.05, 599.28	Glycerophospholipid				✓	
LPC(18:2/0:0)	9.32	564.332	[M-H]-	224.06, 242.08, 279.23, 280.24, 504.31	Glycerophospholipid	✓	✓	✓	✓	✓
PI(18:1/0:0)	10.77	597.306	[M-H]-	152.99, 241.01, 281.24, 417.24, 597.30	Glycerophospholipid		✓		✓	
PE-NME2(18:1/18:1)	11.6	506.29		152.99, 168.00, 224.03, 281.29	Glycerophospholipid			✓	✓	✓
PI(16:0/0:0)	10.63	571.29	[M-H]-	152.99, 223.00, 255.23, 315.04, 571.29	Glycerophospholipid	✓	✓	✓	✓	✓
1-Oleoylglycerophosphoserine	9.52	522.285	[M-H]-	152.99, 171.00, 281.25, 435.25, 522.26	Glycerophospholipid	✓	✓	✓	✓	✓
PE(16:0/0:0)	9.14	452.28	[M-H]-	122.00, 140.01, 152.99, 196.03, 214.04, 255.23, 452.27	Glycerophospholipid	✓	✓	✓	✓	✓
PE(16:1/0:0)	8.79	450.262	[M-H]-	140.01, 152.99, 196.03, 214.04, 253.21	Glycerophospholipid	✓	✓	✓	✓	✓
PE(17:1/0:0)	9.04	464.286	[M-H]-	100.01, 140.01, 152.99, 196.03, 214.04, 267.23	Glycerophospholipid				✓	
PE(18:1/0:0)	9.28	478.295	[M-H]-	122.00, 140.01, 152.99, 196.03, 214.04, 281.24, 478.29	Glycerophospholipid	✓	✓	✓	✓	✓
PE(18:2/0:0)	9	476.282	[M-H]-	122.00, 140.01, 152.99, 196.03, 261.22, 279.23, 476.27	Glycerophospholipid	✓	✓	✓	✓	✓
PE(18:3/0:0)	8.76	474.265	[M-H]-	140.01, 152.99, 196.03, 214.04, 277.22	Glycerophospholipid	✓	✓	✓	✓	✓

PG(16:0/0:0)	10.83	483.274	[M+FA]-	124.85, 152.171.00,227.04, 255.25, 483.27	Glycerophospholipid			✓		
PG(18:1/0:0)	11.24	509.29	[M-H]-	152.99, 227.03, 245.04, 281.27	Glycerophospholipid			✓	✓	
PG(18:2/0:0)	10.15	507.274	[M-H]-	152.99, 227.03, 279.23, 507.27	Glycerophospholipid	✓		✓	✓	✓
PG(19:1/0:0)	8.43	523.27	[M+FA]-	152.99, 183.10, 2227.03, 295.27	Glycerophospholipid			✓		
PI(18:0/0:0)	12.27	599.322	[M-H]-	152.99, 241.01, 283.27, 419.25, 599.31	Glycerophospholipid		✓			
PI(18:2/0:0)	10.3	595.291	[M-H]-	152.95, 171.00, 223.00, 241.01, 279.23, 315.04	Glycerophospholipid	✓	✓	✓	✓	✓
Compound NP-015301	5.6	261.134	[M-H]-	123.08.08, 125.09, 143.10, 169.08, 185.11, 187.09	Fatty acids				✓	
Eicosanoic acid	9.53	311.278	[M-H]-	119.04, 183.01, 197.02, 225.05, 247.20, 311.16	Fatty acids	✓	✓	✓	✓	✓
Turanose	0.72	387.115	[M+FA]-	101.02, 113.02, 119.01, 131.03, 143.03, 149.04, 161.04, 179.05	Fatty acyl glycosides					✓
FA 18:1+3O	6.96	329.234	[M-H]-	127.11, 139.11, 171.10, 183.13, 211.13, 229.14	Fatty acids	✓			✓	
9,10-Dihydroxystearic acid	8.3	315.254	[M-H]-	127.11, 141.12, 155.10, 171.10, 201.11, 297.24, 315.25	Fatty acids	✓				
12_13-DIHOME	7.96	313.239	[M-H]-	111.08, 127.07, 129.09, 183.15, 195.14, 295.22	Fatty acids				✓	
13-HOTrE	7.78	293.213	[M-H]-	177.09, 192, 205.12, 221.15, 236.10	Fatty acids		✓		✓	
16-hydroxypalmitic acid	9.26	271.228	[M-H]-	195.22, 197.19, 221.19, 223.20, 225.22, 253.21	Fatty acids	✓	✓	✓	✓	
2,4-dihydroxyheptadec-16-enyl acetate	7.26	327.218	[M-H]-	119.05, 133.06, 149.10, 170.00, 183.01, 197.02, 225.06, 239.07, 247.20, 327.16	Fatty acids				✓	

9,10-DIHOME	7.84	313.238	[M-H]-	127.11, 171.10, 183.10, 201.11, 277.21, 313.24	Fatty acids		✓			
9,12,13,TriHODE		677.426	2M-2H+Na	233.11, 327.21, 331.18, 349.20	Fatty acids				✓	
9-HOTrE	7.88	293.198	[M-H]-	125.09, 177.09, 192.11, 205.12, 221.10	Fatty acids				✓	
9-KODE	7.21	293.179	[M-H]-	192.11, 205.12, 221.11, 220.14	Fatty acids	✓	✓	✓	✓	✓
FA 18:2+2O		311.223	[M-H]-	125.09, 171.10, 183.01, 209.15, 293.21, 311.17	Fatty acids	✓				
Cembratetraene-16,2:19,6-diolide	7.52	327.164	[M-H]-	119.05, 170.00, 171.10, 183.01, 197.02, 327.16	Prenol lipids	✓	✓	✓	✓	✓
Arteether	8.28	293.213	[M-H2O-H]-	177.09, 192.11, 205.12, 221.15, 236.10, 293.17	Prenol lipids	✓	✓			✓
Miltirone	7.47	283.169	[M+H]+	184.05, 212.04, 240.268.03, 283.06	Prenol lipids			✓		
Aurapten	9.19	297.15	[M-H]-	119.05, 183.01, 197.02, 198.03, 297.15	Benzopyrans		✓			
Thymol-beta-D-glucoside	9.28	311.169	[M-H]-	149.09, 183.01, 197.02, 211.04, 239.07, 267.10, 311.16	Carbohydrates	✓	✓	✓		✓
Andrastin A	7.98	485.255	[M-H]-	167.03, 182.05, 349.21, 397.23, 425.23, 453.22, 485.25	Steroids		✓		✓	
Canrenone	10.99	339.201	[M-H]-	119.04, 183.01, 197.02, 225.05, 239.07, 339.20	Steroids and steroid derivatives	✓	✓	✓	✓	✓
Compound NP-006769	11.93	339.201	[M-H]-	170.00, 183.01, 184.01, 197.02, 339.20	Prenol lipids				✓	✓
Aloe-emodin	6.5	269.046	[M-H]-	182.03, 197.06, 210.03, 225.05, 241.05, 269.04	Anthraquinones			✓		
Emodin	8.2	269.046	[M-H]-	181.06, 197.06, 210.03, 225.05, 241.05, 269.04	Anthraquinones			✓		
Endocrocin	6.5	313.036	[M-H]-	197.06, 225.05, 241.05, 269.04, 295.02, 313.03	Anthracenes			✓		

Fallacinol	6.2	299.057	[M-H]-	227.03, 239.03, 255.03, 256.03, 299.05	Anthraquinones			✓		
Isorhodoptilometrin	7.32	313.072	[M-H]-	197.06, 224.04, 240.04, 268.03, 313.07	Polyketides			✓		
Dodecylbenzenesulfonic acid	11.2	325.185	[M-H]-	170.00, 183.01, 197.02, 261.22, 325.18	Organosulfonic acid	✓	✓	✓	✓	✓
APS-2-79	8.87	386.198	[M-H]-	250.15, 310.18, 328.10, 356.10	Benzene and substituted derivatives	✓				
Asterric acid	6.55	347.078	[M-H]-	105.03, 149.02, 212.04, 256.03, 297.04, 297.04	Benzene and substituted derivatives	✓		✓		
C10-Dialkyl tetralin sulfonate	8.44	295.138	[M-H]-	210.03, 223.04, 237.05, 251.07, 295.13	Benzene and substituted derivatives	✓				
Decylbenzenesulfonic acid	9.03	297.154	[M-H]-	119.04, 170.00, 183.01, 198.03, 239.07, 281.15, 297.15	Benzene and substituted derivatives	✓	✓	✓	✓	✓
Dihydrobenzoic acid pentose	2.34	285.063	[M-H]-	108.02, 109.02, 151.00, 152.01, 153.01	Carbohydrates			✓		
Metazachlor	4.09	278.067	[M+H]+	105.03, 106.04, 132.04, 133.05	Benzene and substituted derivatives	✓				
3-O-Demethylsulochrin	5.48	317.067	[M-H]-	105.03, 123.04, 149.02, 167.03, 197.06, 241.04, 299.05	Benzene and substituted derivatives			✓		
Methyl asterrate	6.64	407.099	M+FA-H	197.06, 211.04, 225.05, 254.05, 270.05, 329.06, 361.09	Benzene and substituted derivatives			✓		
Sulochrin	5.99	331.083	[M-H]-	105.03, 122.03, 149.02, 166.02, 240.04, 299.05	Benzene and substituted derivatives	✓	✓	✓		
6-(4-sulfophenyl)decanoic acid	7.48	327.165	[M-H]-	170.00, 183.01, 184.02, 197.02, 309.15	Benzene and substituted derivatives		✓	✓		
39674-97-0	7.47	240.043	[M-H]-	184.05, 197.02, 211.03, 212.04, 240.04	Indoles			✓		
Benzoic acid + 2O, O-Hex	2.14	315.101	[M-H]-	108.02, 109.02, 152.01, 153.01	Carbohydrates					✓
Hexosyl LPE 16:0	9.01	614.317	[M-H]-	152.99, 238.05, 255.23, 452.27,	Carbohydrates		✓	✓		✓

				494.29, 524.30, 614.33						
Hexosyl LPE 18:2	8.75	638.334	[M-H]-	214.04, 268.05, 279.23, 476.27, 638.33	Carbohydrates		✓	✓	✓	✓
Hexosyl LPE 18:3	8.62	636.323	[M-H]-	196.03, 214.04, 277.21, 474.27, 636.31	Carbohydrates		✓	✓	✓	✓
Megxp0_000647	2.29	397.159	[M-H]-	191.11, 220.09, 235.06	Carbohydrates		✓		✓	
Gentiopicroside	7.15	357.142	[M+H]+	121.06, 133.06, 149.06, 177.05, 195.06	Carbohydrates			✓		
RAFFINOSE	0.69	549.17	[M+FA]-	179.05, 323.09, 341.11, 503.16	Carbohydrates			✓		
Sucrose	0.72	387.114	[M+FA]-	113.02, 119.03, 143.03, 179.05, 341.11	Carbohydrates	✓				✓
Melibiose, pure	0.73	387.115	[M+FA]-	101.02, 119.03, 143.03, 161.04, 179.05, 221.06, 341.10	Carbohydrates			✓		
EMBELIN	9.91	293.179	[M-H]-	192.11, 205.12, 221.15, 236.10, 293.17	Carbohydrates					✓
5,6,2'-Trimethoxyflavone	9.73	311.096	[M-H]-	119.04, 149.09, 183.01, 212.05, 225.05, 311.16	Flavonoids	✓	✓	✓	✓	✓
5-hydroxy-6,7-dimethoxyflavone	9	297.084	[M-H]-	119.04, 170.00, 183.01, 197.02, 225.05, 239.03, 297.08	Flavonoids	✓	✓	✓	✓	✓
Gardenin B	6.31	359.078	[M+H]+	297.04, 298.04, 311.05, 329.06	Flavonoids		✓			
5-O-Methylgenistein	7.48	283.062	[M-H]-	184.05, 212.04, 240.04, 268.03, 283.06	Isoflavonoids			✓		
Derrustone	10.36	325.108	[M-H]-	119.05, 170.00, 183.01, 197.02, 225.05, 239.07, 325.18	Isoflavonoids	✓	✓	✓	✓	✓
Hesperetin 7-O-rutinoside	5.58	609.196	[M-H]-	125.02, 242.05, 301.07, 325.07	Carbohydrates					✓
3_phenyllactic_acid	4.91	353.113	2M-2H+Na	103.05, 119.04, 147.04, 165.05	Phenylpropanoic acids	✓	✓	✓	✓	✓
Compound NP-015327	7.06	313.151	[M-H]-	119.05, 170.00, 183.01, 197.02, 313.14	Coumarins and derivatives				✓	

Pd-Ib	8.01	341.106	[M-H]-	119.04, 170.00, 183.01, 197.02, 239.07, 341.17	Coumarins and derivatives	✓	✓	✓	✓	✓
Rosmarinic acid	5.51	359.1	[M-H]-	123.04, 133.02, 135.04, 161.02, 179.03	Cinnamic acids and derivatives		✓			
Pannaric acid	6.49	315.045	[M-H]-	199.06, 227.06, 243.05, 256.03, 256.03, 271.06, 315	Dibenzofurans			✓		
4-Hydroxyvertixanthone	5.99	299.057	[M-H]-	183.04, 212.04, 240.04, 267.03, 299.05	Phenols	✓		✓		
4,6-Dimethoxy-1-methyl-1H-indole-2-carboxylic acid	7.21	236.106	[M+H]	134.03, 148.05, 177.07, 192.11	Indoles and derivatives	✓	✓	✓		
Roquefortine C	6.1	388.183	[M-H]-	123.01, 134.03, 147.04, 190.04, 203.05, 318.09, 38.17	Indoles and derivatives	✓	✓		✓	✓
Tryptophan	2.31	407.155	2M-H	116.05, 142.06, 159.09, 203.08, 225.06	Indoles and derivatives	✓	✓	✓	✓	✓
	2.17	206.034	[M-H]-	116.05, 118.02, 144.04, 146.02	Indoles and derivatives		✓			✓
Ropivacaine	7.17	309.203	[M+Cl]-	152.08, 190.09, 209.15, 265.18, 309.17	Carboxylic acids and derivatives			✓		
Riboflavin	4.95	375.137	[M-H]-	144.07, 157.08, 169.07, 184, 212.08, 241.07, 255.08	Flavin nucleotides	✓	✓	✓	✓	✓
Compound NP-007926	5.82	432.182	[M-H]-	177.04, 276.08, 304.08, 332.07, 342.13, 384.15	Indoles and derivatives	✓	✓		✓	✓
CJ-21058	9.36	386.235	[M-H]-	124.00, 285.18, 312.23, 356.22, 386.23	Naphthalenes	✓				
Equisetin	9.12	372.219	[M-H]-	124.00, 138.01, 152.03, 167.05, 260.16, 298.21, 324.19, 342.20, 372.21	Naphthalenes	✓		✓		
Guanosine-3',5'-cyclic monophosphate	0.97	344.053	[M+H]	107.03, 108.02, 133.01, 150.04	Purine nucleotides	✓	✓	✓	✓	✓
Nicotinamide Adenosine Dinucleotide	1	664.107	[M-H]-	272.95, 328.04, 346.05, 397.02, 408.01	Adenine Nucleotides	✓	✓		✓	✓

Flavin adenine dinucleotide	4.44	784.152	[M-H]-	180.99, 346.05, 437.08, 517.05, 784.15	Flavin nucleotides	✓	✓	✓	✓	✓
2'-Deoxyadenosine	1.1	266.09	[M-H]-	107.03, 133.03, 134.04, 160.06	Deoxyribonucleosides	✓	✓			✓
2-O-Methylguanosine	1.56	296.1	[M-H]-	106.02, 121.05, 133.01, 149.03, 164.05	Purine Nucleosides	✓				
Adenosine	1.11	312.065		107.03, 134.04, 266.09, 134.11	Purine Nucleosides	✓	✓	✓	✓	✓
Adenosine 5'-diphosphate	0.91	426.023	[M-H]-	134.04, 158.92, 272.95, 328.04, 408.	Adenine Nucleotides	✓	✓	✓	✓	✓
Guanosine	1.08	282.077	[M-H]-	107.03, 108.02, 133.01, 150.04	Purine Nucleosides			✓	✓	✓
Guanosine monophosphate	0.86	362.055	[M-H]-	120.96, 150.04, 152.99, 192.99, 211.00	Guanine Nucleotides				✓	✓
UDP-glucose	0.64	565.05	[M-H]-	138.98, 241.01, 272.95, 323.02, 384.98, 565.04	Nucleoside Diphosphate Sugars	✓	✓	✓	✓	✓
UPD-alpha-D-Galactose	0.88	565.049		158.92, 211.00, 241.01, 272.95, 305.02, 323.02, 384.98	Pyrimidine nucleotides	✓	✓	✓	✓	✓
Uridine 5'-diphospho-N-acetylglucosamine	0.65	606.076	[M-H]-	158.92, 272.95, 323.02, 362.00, 384.98, 606.07	Pyrimidine nucleotides	✓	✓	✓	✓	✓
Supiculisporic Acid	7.87	327.199	[M-H]-	124.01, 221.18, 239.20, 265.18, 327.16	Carbonyl compound		✓		✓	
EleutherazineB	4.65	451.242	[M-H]-	110.06, 167.11, 210.12, 227.15, 249.16, 266.18, 309.19, 339.20, 391.23	Piperazines				✓	✓
Compound NP-008285	9.9	325.109	[M-H]-	119.04, 170.00, 183.01, 197.02, 212.05, 225.05, 253.09, 261.22, 325.18	Carboxylic acids and derivatives	✓	✓	✓		✓
Compound NP-005913	7.2	294.18	[M-H]-	178.09, 193.11, 205.12, 218.09, 220.14, 221.15, 237.10	Carboxylic acids and derivatives			✓		
Compound NP-008689	6.66	511.199	[M-H]-	118.06, 124.02, 164,.07, 189.10, 215.08, 233.09, 259.08, 329.23	Carboxylic acids and derivatives				✓	

L-Aspartyl-L-phenylalanine	3.56	279.1	[M-H]-	103.05, 113.126.04, 147.04, 175.08, 200.07, 217.09	Dipeptides	✓	✓	✓	✓	✓
Carbamylcholine	8.49	293.213	[2M-2H2O+Cl]-	205.12, 220.14, 221.15, 236.10, 293.21	Carboxylic acids and derivatives		✓	✓		
CHEMBL446487	5.09	264.088	[M-H]-	103.05, 111.03, 147.04, 156.08, 164.07, 184.07,202.08	Carboxylic acids and derivatives	✓	✓	✓	✓	✓
Diprotin A	5.01	340.221	[M-H]-	130.08.155.11, 183.14, 209.12, 227.14	Oligopeptides			✓		
Eim08-13459	5.64	365.172	[M-H]-	146.08, 147.04, 164.07, 218.08	Carboxylic acids and derivatives					✓
Glutamylphenylalanine	0.64	293.136	[M-H]-	101.02, 113.07, 131.07, 143.08, 173.09	Oligopeptides		✓	✓	✓	✓
Gamma-Glutamylphenylalanine	3.86	293.11	[M-H]-	103.05, 109.04, 122.04, 128.03, 147.04, 164.07	Oligopeptides	✓	✓		✓	
Leucyl-phenylalanine	4.66	277.138	[M-H]-	103.05, 129.10, 147.04, 164.07	Oligopeptides				✓	
L-valyl-L-phenylalanine	3.95	263.141	[M-H]-	103.05, 115.08, 147.04, 164.06	Oligopeptides				✓	
N-Acetyl-L-tyrosine	3.14	222.077	[M-H]-	107.04, 119.04, 163.03, 180.06	Carboxylic acids and derivatives	✓	✓	✓		✓
Oglufanide	5.05	314.113	[M-H2O-H]-	109.04, 116.05, 127.05, 141.06, 185.05,	Oligopeptides	✓	✓	✓	✓	✓
Oxiglutatione	0.79	611.148	[M-H]-	143.04, 128.03, 210.08, 254.07, 272.08, 306.07	Oligopeptides	✓	✓	✓	✓	✓
Pantethine	5.32	589.218	[M+Cl]-	128.01, 130.03, 146.08, 217.11, 275.10, 277.12	Carboxylic acids and derivatives		✓	✓		✓
L-valyl-L-tyrosine	1.54	279.132	[M-H]-	107.04, 115.08, 119.05, 129.10, 279.13	Oligopeptides	✓				
DL-3-Phenyllactic acid	4.9	165.057	2M-H	101.03, 103.05, 117.03, 119.05	Benzene and substituted derivatives		✓			✓
Phenampromide	7.28	309.175	[M+Cl]-	151.04, 152.08, 209.15, 252.10, 265.17, 309.16	Alkaloid	✓				
R-N6-succinyladenosine	2.21	382.101	[M-H]-	115.00, 134.04, 162.07, 206.06,	Purine Nucleosides	✓	✓	✓	✓	✓

				250.05, 266.09, 382.10						
2-(3-carboxypropanoylamino)hexanoic acid	4.84	461.207	2M-H	111.03, 130.08, 142.12, 168.10, 212.09, 230.10	Carboxylic acids and derivatives				✓	
Megxm0_000076	5.5	305.151	[M-H]-	103.05, 116.07, 127.08, 131.04, 147.04, 188.07, 202.12, 263.13	Dipeptide derivative	✓			✓	
HYDROQUINIDINE	10.9	325.1865	[M-H]-	183.01, 184.01, 197.02, 198.03, 309.11, 325.18	Alkaloids	✓	✓	✓	✓	✓
Ingenol	6.38	383.209	[M+Cl]-	187.09, 205.19, 311.22, 329.23, 347.18, 383.20	Prenol lipids		✓	✓	✓	✓
P_hydroxyphenyl_lactic_acid	2.66	363.13	2M-H	119.05, 135.04, 163.03, 181.05, 203.03	Phenolic acid derivatives	✓				✓