Table S1 Reported compounds of *Ophiocordyceps sinensis*.

Number	Category	Compound name	Molecular formula	Molecular weight	References
1	Others	Diacylglycerol	C37H70O5	594.95	[1]
2	Others	Phosphatidyl cholines	C10H21NO8P	314.25	[1]
3	Others	myriocin	C21H39NO6	401.54	[2]
4	Others	3-Prop-2-enylidenecyclobutene Olefine	C7H8	92.14	[3]
5	Others	2-Methyl cyclopentanol Alcohol	C6H12O	100.16	[3]
6	Others	Methyl carbamate Others	C2H5NO2	75.07	[3]
7	Others	4-Methyl pyrimidine Others	C5H6N2	94.11	[3]
8	Others	o-Xylene 5.09hydrocarbon	C8H10	106.16	[3]
9	Others	2,2-Dimethoxy ethanol Alcohol	C4H10O3	106.12	[3]
10	Others	N-methoxy formamide Others	C2H5NO2	75.07	[3]
11	Others	2-Methyl cyclopentanone Ketone	C6H10O	98.14	[3]
12	Others	4,6-Dimethyl pyrimidine, Others	C6H8N2	108.14	[3]
13	Others	4-Carene Terpenes	C10H16	136.23	[3]
14	Others	(2,5-Dimethyloxan-2-yl) methanol Alcohol	C8H16O2	144.21	[3]
15	Others	1-Phenyl-1,2-propanedione Ketone	C9H8O2	148.16	[3]
16	Others	Sabinene Terpenes	C10H16	136.23	[3]
17	Others	6-Ethenyl-2,2,6-trimethyloxan-3-one Ketone	C10H16O2	168.23	[3]
18	Others	(4-Hydroxyphenyl) phosphonic acid Others	C6H7O4P	174.09	[3]
19	Others	(−)-β-Pinene Terpenes	C10H16	136.23	[3]
20	Others	1,2,3-Trimethyl benzene 0.67hydrocarbon	C9H12	120.19	[3]
21	Others	3-Carene Terpenes	C10H16	136.23	[3]
22	Others	2,5,6-Trimethyl decane Alkane	C13H28	184.36	[3]
23	Others	2,6,7-Trimethyl decane Alkane	C13H28	184.36	[3]
24	Others	o-Cymene 0.21hydrocarbon	C10H14	134.22	[3]

25	Others	2,4-Dimethyl-2,3-heptadien-5-yne Olefine	C9H12	20.19	[3]
26	Others	D-Limonene Terpenes	C12H26	170.33	[3]
27	Others	2,2,4,4-Tetramethyl octane Alkane	C10H16	136.23	[3]
28	Others	2,5,9-Trimethyl decane Alkane	C13H28	184.36	[3]
29	Others	2,3-Dihydro pyran-6-one Ketone	C5H6O2	98.1	[3]
30	Others	3-Octene-2-one Ketone	C8H14O	126.2	[3]
31	Others	2,7,10-Trimethyl dodecane Alkane	C15H32	212.41	[3]
32	Others	2-Propyl toluene 5.72hydrocarbon	C10H14	134.22	[3]
33	Others	2-Ethyl-1,4-dimethyl benzene 0.00hydrocarbon	C10H14	134.22	[3]
34	Others	2,4,6-Trimethyl decane Alkane	C13H28	184.36	[3]
35	Others	Phenylglyoxyl monohydrate Others	C8H8O3	152.15	[3]
36	Others	3,5-Octadien-2-one Ketone	C8H12O	124.18	[3]
37	Others	2,6-Dimethyl-6-trifluoroacetoxyoctane Others	C12H21F3O2	254.29	[3]
38	Others	1,3-Dimethyl-3-ethyl benzene 0.24hydrocarbon	C10H14	134.22	[3]
39	Others	Piperityl acetate Others	C12H20O2	196.29	[3]
40	Others	1,2,4,5-Tetramethyl benzene	C10H14	134.22	[3]
41	Others	1,2-Dimethoxyethyl benzene	C10H14O2	166.22	[3]
42	Others	Dodecane,2,6,11-trimethyl	C15H32	212.41	[3]
43	Others	4,5-Dimethylnonane	C11H24	156.31	[3]
44	Others	Linalool	C10H18O	154.25	[3]
45	Others	2-Nonen-1-ol	C9H18O	142.24	[3]
46	Others	1,2,3,5-Tetramethyl benzene	C10H14	134.22	[3]
47	Others	6-Ethyl-2-methyl octane	C11H24	156.31	[3]
48	Others	1,5,6,7-TetramethylC4 5 0.00bicyclo[3.2.0]hept a-2,6-diene	C11H16	148.24	[3]

49	Others	AromaticC46 1,2,3,4-Tetramethyl benzene	C10H14	134.22	[3]
50	Others	AromaticC47 3,5-Diethyl-1-methyl benzene	C11H16	148.24	[3]
51	Others	4-Methyl indane	C10H12	132.2	[3]
52	Others	1,4-Diethyl-2-methyl benzene	C11H16	148.24	[3]
53	Others	1,2,3,4-Tetramethyl fulvene	C10H14	134.22	[3]
54	Others	[but-2-en-2-yl]Benzene	C10H12	132.2	[3]
55	Others	2,3-Dimethyl decane	C12H26	170.33	[3]
56	Others	4’-Methyl propiophenone	C10H12O	148.2	[3]
57	Others	5-Butan-2-ylnonane	C13H28	184.36	[3]
58	Others	9-Methyl heptadecane	C18H38	254.49	[3]
59	Others	3-Methyl undecane	C12H26	170.33	[3]
60	Others	1-Ethyl-2,4,5-trimethyl benzene	C11H16	148.24	[3]
61	Others	1-Methyl-cyclododecene	C13H24	180.33	[3]
62	Others	3,7,11-Trimethyl dodecan-1-ol	C15H32O	228.41	[3]
63	Others	Dodecane	C12H26	170.33	[3]
64	Others	(+)-α-Terpineol	C10H18O	154.25	[3]
65	Others	3,4-Dimethyl cumene	C11H16	148.24	[3]
66	Others	4,7-Dimethyl undecane	C13H28	184.36	[3]
67	Others	Cyclodecanol	C10H20O	156.26	[3]
68	Others	2,6-Dimethyl undecane	C13H28	184.36	[3]
69	Others	2,4-Dimethyl acetophenone	C10H12O	148.2	[3]
70	Others	2-Hydroxycineole	C10H18O2	170.25	[3]
71	Others	2,8-Dimethyl undecane	C13H28	184.36	[3]
72	Others	2,6-Dimethyl benzaldehyde	C9H10O	134.17	[3]
73	Others	2-Hydroxycineol	C10H18O2	170.25	[3]
74	Others	Thieno[2,2,3]pyridine	C7H5NS	135.19	[3]
75	Others	3-Hydroxy cineole	C10H18O2	170.25	[3]
76	Others	4-Methyl dodecane	C13H28	184.36	[3]
77	Others	1,3-Di-tert-butyl benzene	C14H22	190.32	[3]
78	Others	4,7-Dimethyl indan	C11H14	146.23	[3]
79	Others	2,3-Dimethyl undecane	C13H28	184.36	[3]
80	Others	2,4-Dimethyl dodecane	C14H30	198.39	[3]
81	Others	2,6,11-Trimethyl	C15H32	212.41	[3]

		dodecane			
82	Others	2,3,4-Trimethyl dodecane	C13H28	184.36	[3]
83	Others	1,5,6,7-Tetramethylbicyclo[3.2.0]hepta-C80 0.002,6-diene	C11H16	148.24	[3]
84	Others	1,7,7-Trimethylbicyclo[2.2.1]heptan-C81 0.002-yl acetate	C12H20O2	196.29	[3]
85	Others	2-Undecanone	C11H22O	170.29	[3]
86	Others	Tridecane	C13H28	184.36	[3]
87	Others	4,6-Dimethyl dodecane	C14H30	198.39	[3]
88	Others	1-Methyl naphthalene	C11H10	142.2	[3]
89	Others	2,3,5,8-Tetramethyl decane	C14H30	198.39	[3]
90	Others	α-Methyl-1H-indene-1-methanol acetate	C13H14O2	202.25	[3]
91	Others	2,7,10-Trimethyl dodecane	C15H32	212.41	[3]
92	Others	Silphiperfol-5-ene	C15H24	204.35	[3]
93	Others	4-Ethyl undecane	C13H28	184.36	[3]
94	Others	Silphinene	C15H24	204.35	[3]
95	Others	2,3-Dimethyl dodecane	C14H30	198.39	[3]
96	Others	α-Longipinene	C15H24	204.35	[3]
97	Others	farnesane	C15H32	212.41	[3]
98	Others	(+)-Cyclosativene	C15H24	204.35	[3]
99	Others	Modephene	C15H24	204.35	[3]
100	Others	Tetradecane	C14H30	198.39	[3]
101	Others	α-Isocomene	C15H24	204.35	[3]
102	Others	(-)-α-Gurjunene	C15H24	204.35	[3]
103	Others	2,6-Dimethyl heptadecane	C19H40	268.52	[3]
104	Others	β-Maaliene	C15H24	204.35	[3]
105	Others	(-)-Aristolene	C15H24	204.35	[3]
106	Others	2-Isopropyl-5-methyl-9-Hmethylene[4.4.0]dec-1-ene	C15H24	204.35	[3]
107	Others	α-Bergamotene	C15H24	204.35	[3]
108	Others	Isoledene	C15H24	204.35	[3]
109	Others	Guaia-3,9-diene	C15H24	204.35	[3]
110	Others	2,10-Dimethyl heptadecane	C19H40	268.52	[3]
111	Others	Seychellene	C15H24	204.35	[3]
112	Others	2,6-Di-tert-butyl-4-methyl-p-quinol	C15H24O2	236.35	[3]
113	Others	Pentadecane	C15H32	212.41	[3]

114	Others	(+)-Valencene	C15H24	204.35	[3]
115	Others	β-Sesquiphellandrene	C15H24	204.35	[3]
116	Others	1-Iodo-2-methyl undecane	C12H25	169.33	[3]
117	Others	α-Bulnesene	C15H24	204.35	[3]
118	Others	2,4-Di-tert-butyl phenol	C14H22O	206.32	[3]
119	Others	2,4-Di-tert-butyl-6-methyl phenol	C15H24O	220.35	[3]
120	Others	(+)-Cuparene	C15H22	202.33	[3]
121	Others	Hexadecane	C16H34	226.44	[3]
122	Others	2,6-Di-tert-butyl-4-sec-butyl phenol	C18H30O	262.43	[3]
123	Others	Pristane	C19H40	268.52	[3]
124	Others	2,3-Dihydroxybenzoic acid	C7H6O4	154.12	[4]
125	Others	4-Hydroxyphenylacetic acid	C8H8O3	152.15	[4]
126	Others	Benzoic acid	C7H6O2	122.12	[4]
127	Others	Dihydroergovalined	C29H37N5O5	535.63	[4]
128	Others	Dihydroergonine	C30H39N5O5	549.66	[4]
129	Others	Dihydroergocornine	C31H41N5O5	563.69	[4]
130	Others	Dihydroergotamine	C33H37N5O5	583.68	[4]
131	Others	2-Aminooctadec-4-ene-1,3,4-triol	C18H37NO3	315.49	[4]
132	Others	9,12,13-Trihydroxyoctadec-11-enoic acid	C18H34O5	330.46	[4]
133	Others	2-Amino-1,3,4-octadecanetriol	C18H39NO3	317.51	[4]
134	Others	Cycloaspeptide C	C35H41N5O6	627.73	[4]
135	Others	Octadecanedioic acid or isomer	C18H34O4	314.46	[4]
136	Others	Dihydroergocristine	C35H41N5O5	611.73	[4]
137	Others	2-Amino-1,3-docosanediolc	C22H47NO2	357.61	[4]
138	Others	2-Amino-1,3,4-docosanetriol	C22H47NO3	373.61	[4]
139	Others	2,3-Dihydroxyoctadecanoic acidc	C18H36O4	316.47	[4]
140	Others	13-Hydroxy-6Z,9Z,11E-octadecatrienoic acid or isomer	C18H30O3	294.43	[4]
141	Others	9-Hydroxy-10,12-octadecadienoicacid or isomer	C18H32O3	296.44	[4]
142	Others	15,18,21,24-Triacontat	C30H52O2	444.73	[4]

		etraenoicacid			
143	Others	Linolenic acid or isomer	C18H32O2	280.44	[4]
144	Others	3-Oxooctadecanoic acidc	C18H34O3	298.46	[4]
145	Others	3-Hydroxy-6Z,9Z,11E-octadecatrienoic acid or isomerc	C18H30O3	294.43	[4]
146	Others	3-Oxopalmitic acid	C16H30O3	270.41	[4]
147	Others	2-Hydroxyhexadecanoic acid	C16H32O3	272.42	[4]
148	Others	n-Linoleoylsarcosine	C21H37NO3	351.52	[4]
149	Others	Linoleamide	C18H33NO	279.46	[4]
150	Others	2-Hydroxyoctadecanoic acid or isomer	C18H36O3	300.48	[4]
151	Others	Glycerol 1-monolinolate	C21H38O4	354.52	[4]
152	Others	Sphingosine	C18H37NO2	299.49	[4]
153	Others	Palmitoleic acid	C16H30O2	254.41	[4]
154	Others	2-Monopalmitin or isomer	C19H38O4	330.5	[4]
155	Others	Diethylene glycol monoricinoleate	C22H42O5	386.56	[4]
156	Others	Hexadecanoic acid, 2,3-dihydroxypropyl ester	C19H38O4	330.5	[4]
157	Others	Barogenin	C27H42O4	430.62	[4]
158	Others	Hexadecanamide	C16H33NO	255.44	[4]
159	Others	Linoleic acid or isomer	C18H32O2	280.44	[4]
160	Others	2-Monopalmitin or isomer	C19H38O4	330.5	[4]
161	Others	Glyceryl monooleate	C18H32O2	280.33	[4]
162	Others	N-[(9Z,12Z)-9,12-Octadecadienoyl] leucine	C24H43NO3	393.6	[4]
163	Others	Palmitic acid	C16H32O2	256.42	[4]
164	Others	2-Hydroxyoctadecanoic acid or isomer	C18H36O3	300.48	[4]
165	Others	N-Palmitoyl-leucine	C22H43NO3	369.58	[4]
166	Others	Oleic acidc	C18H34O2	282.46	[4]
167	Others	Ethyl linoleate	C20H36O2	308.5	[4]
168	Others	2,3-Dihydroxypropyl stearate	C21H42O4	358.55	[4]
169	Others	Docosanedioic acid	C22H42O4	370.56	[4]
170	Others	Stearoyl ceramide	C36H71NO3	565.95	[4]
171	Others	11,14-Eicosadienoicacid	C20H36O2	308.5	[4]

172	Others	Stearic acid	C18H36O2	284.48	[4]
173	Others	9-Tricosenamide	C23H45NO	351.61	[4]
174	Others	11-Eicosenoic acid	C20H38O2	310.51	[4]
175	Others	2-Hydroxydocosanoic acid or isomerc	C22H44O3	356.58	[4]
176	Others	Diethanollinoleic amidec	C22H43NO	337.58	[4]
177	Others	Ethyl oleate	C20H38O2	310.51	[4]
178	Others	2- Hydroxydocosanoic acid or isomerc	C22H44O3	356.58	[4]
179	Others	Tricosenamide	C23H47NO	353.62	[4]
180	Others	Ergosta-7,22-diene-3,5,6-triol	C28H46O3	430.66	[4]
181	Others	2-Hydroxydocosanoic acid or isomerc	C22H44O3	356.58	[4]
182	Others	2-Hydroxy lignoceric acid	C23H46O3	370.61	[4]
183	Others	Ergosterol	C28H44O	396.65	[4]
184	Others	1-Pentadecanoyl-2-(9Z-octadecenoyl)-sn-glycerol	C38H74O8	658.99	[4]
185	Others	Glyceryl dilinoleatec	C39H68O5	616.95	[4]
186	Others	1-Palmitoyl-2-linoleoyl-sn-glycerol	C37H68O5	592.93	[4]
187	Others	1-Oleoyl-2-linoleoyl-rac-glycerol or isomer	C39H70O5	618.97	[4]
188	Others	2-Hydroxy-N-1,3,4-trihydroxy-octadecanamide	C42H85NO5	684.12	[4]
189	Others	Glycerol dioleate or isomer	C39H72O5	620.98	[4]
190	Others	Acetylacetone	C5H8O2	100.12	[5]
191	Others	N, N-Dimethylglycine	C4H9NO2	103.12	[5]
192	Others	Methoxyimino-acetic acid	C3H5NO3	103.08	[5]
193	Others	Boric acid	H3BO3	61.83	[5]
194	Others	2,3,6-Trimethyl-pyridine	C8H11N	121.18	[5]
195	Others	tert- Butyl carbamate	C5H11NO2	117.15	[5]
196	Others	2-Methoxyimino-propionic acid	C4H7NO3	117.1	[5]
197	Others	Diethyl-carbamic acid	C5H11NO2	117.15	[5]
198	Others	Lactic Acid .	C3H6O3	90.08	[5]
199	Others	Butanedioic acid, dimethyl ester	C6H10O4	146.14	[5]
200	Others	Glycolic acid	C2H4O3	76.05	[5]

201	Others	L-Valine	C5H11NO2	117.15	[5]
202	Others	L-Alanine	C3H7NO2	89.09	[5]
203	Others	Glycine	C2H5NO2	75.07	[5]
204	Others	3-Pyridinol	C5H5NO	95.1	[5]
205	Others	3-Mercapto-propionic acid	C3H6O2S	106.14	[5]
206	Others	4-Pyridinol	C5H5NO	95.1	[5]
207	Others	3-Hydroxy-2-methyl-propionic acid	C4H8O3	104.1	[5]
208	Others	2-Aminobutanoic acid	C4H9NO2	103.12	[5]
209	Others	Phosphoric acid monomethyl ester	CH5O4P	112.02	[5]
210	Others	3- Aminoisobutyric acid	C4H9NO2	103.12	[5]
211	Others	4-Hydroxybutanoic acid	C4H8O3	104.1	[5]
212	Others	2-Amino 3-methyl-butyric acid	C5H11NO2	117.15	[5]
213	Others	L-Serine	C3H7NO2	89.09	[5]
214	Others	Ethanolamine	C2H7NO	61.08	[5]
215	Others	L-Leucine	C6H13NO2	131.17	[5]
216	Others	Glycerol	C3H8O3	92.09	[5]
217	Others	Niacin	C6H5NO2	123.11	[5]
218	Others	L-Proline	C5H9NO2	115.13	[5]
219	Others	Glyceric acid	C3H6O4	106.08	[5]
220	Others	Uracil	C4H4N2O2	112.09	[5]
221	Others	E-2-Butenedioic acid	C4H4O4	116.07	[5]
222	Others	DL-Serine	C3H7NO3	105.09	[5]
223	Others	Isopropyl formate	C4H8O2	88.1	[5]
224	Others	L-Threonine	C4H9NO3	119.12	[5]
225	Others	Pentanedioic acid	C5H8O4	132.11	[5]
226	Others	L-Methionine	C5H11NO2S	149.21	[5]
227	Others	β-Alanine	C3H7NO2	89.09	[5]
228	Others	2,2'-Bipyridine	C10H8N2	156.18	[5]
229	Others	Homoserine	C4H9NO3	119.12	[5]
230	Others	3-Amino-2-piperidone	C5H10N2O	114.15	[5]
231	Others	Aminomalonic acid	C3H5NO4	119.08	[5]
232	Others	DL-malic acid	C4H6O5	134.09	[5]
233	Others	Erythritol	C4H10O4	122.12	[5]
234	Others	L-Aspartic acid	C4H7NO4	133.1	[5]
235	Others	L-5-Oxoproline	C5H9NO3	131.13	[5]
236	Others	4-Aminobutanoic acid	C4H9NO2	103.12	[5]
237	Others	DL-Phenylalanine	C9H11NO2	165.19	[5]
238	Others	Cysteine	C3H7NO2S	121.16	[5]
239	Others	2,3,4-Trihydroxy-butanoic acid	C4H8O5	136.1	[5]

240	Others	2-Hydroxyglutaric acid	C5H8O5	148.11	[5]
241	Others	L-Asparagine	C4H8N2O3	132.12	[5]
242	Others	Pipecolic acid	C6H11NO2	129.16	[5]
243	Others	L-Omithine	C5H12N2O2	132.16	[5]
244	Others	L-Glutamic acid	C5H9NO4	147.13	[5]
245	Others	L-Phenylalanine	C9H11NO2	165.19	[5]
246	Others	3,4,5-Trihydroxy-pentanoic acid	C5H10O5	150.13	[5]
247	Others	Asparagine	C4H8N2O3	132.12	[5]
248	Others	2,3,4,5-Tetrahydroxy-pentanal O-ethy-oxime	C7H15NO5	193.2	[5]
249	Others	2-Aminoadipic acid	C6H11NO4	161.16	[5]
250	Others	Xylitol .	C5H12O5	152.15	[5]
251	Others	Putrescine	C4H12N2	88.15	[5]
252	Others	Aconitic acid	C6H6O6	174.11	[5]
253	Others	DL-Omithine	C5H12N2O2	132.16	[5]
254	Others	Phosphoric acid mono-(2,3-dihydroxy-propyl) ester	C3H9O6P	172.07	[5]
255	Others	L-Glutamine	C5H10N2O3	146.14	[5]
256	Others	Terephthalic acid	C8H6O4	166.13	[5]
257	Others	3,4,5,6-Terahydroxy-2-oxo-hexanoacid	C6H15O7	199.18	[5]
258	Others	Phosphorylethanolamine	C2H8NO4P	141.06	[5]
259	Others	9H-Purin-6-ol	C5H4N4O	136.11	[5]
260	Others	Citric acid	C6H8O7	192.12	[5]
261	Others	Myristic acid	C14H28O2	228.37	[5]
262	Others	Cadaverine	C5H14N2	102.18	[5]
263	Others	DL-tyrosine	C9H11NO3	181.19	[5]
264	Others	D-Fructose	C6H15NO6	197.19	[5]
265	Others	d-Glucose	C6H12O6	180.16	[5]
266	Others	Galactopyranose	C6H12O6	180.16	[5]
267	Others	D-Allose	C7H15NO6	209.2	[5]
268	Others	L-Lysine	C6H14N2O2	146.19	[5]
269	Others	L-Histidine	C6H9N3O2	155.15	[5]
270	Others	L-Tyrosine	C3H11NO3	109.12	[5]
271	Others	Glucopyranose	C6H12O6	180.16	[5]
272	Others	9-Hexadecenoic acid	C16H30O2	254.41	[5]
273	Others	D-Gluconic acid	C6H12O7	196.15	[5]
274	Others	Palmitic Acid	C16H32O2	256.42	[5]
275	Others	Scyllo-Inositol	C6H12O6	180.16	[5]
276	Others	Ferulic acid .	C10H10O4	194.18	[5]
277	Others	Lanthionine	C6H12N2O4S	208.24	[5]
278	Others	Myo-Inositol	C6H12O6	180.16	[5]
279	Others	Linoleic acid	C18H32O2	280.44	[5]

280	Others	Kynurenine	C10H12N2O3	208.21	[5]
281	Others	Oleic acid	C18H34O2	282.46	[5]
282	Others	Cystathionine	C7H14N2O4S	222.26	[5]
283	Others	Stearic acid	C18H36O2	284.48	[5]
284	Others	L-Tryptophan	C11H12N2O2	204.22	[5]
285	Others	D-Glucitol	C6H10O4	146.14	[5]
286	Others	Adenosine	C10H13ON5O4	283.24	[5]
287	Others	Sucrose	C12H22O11	342.3	[5]

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