

## Supplementary information

### Unraveling the Alteration of Chemical Compositions in Cordyceps and Its Host Larvae Using Mass Spectrometry Imaging

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## Supplementary Figure

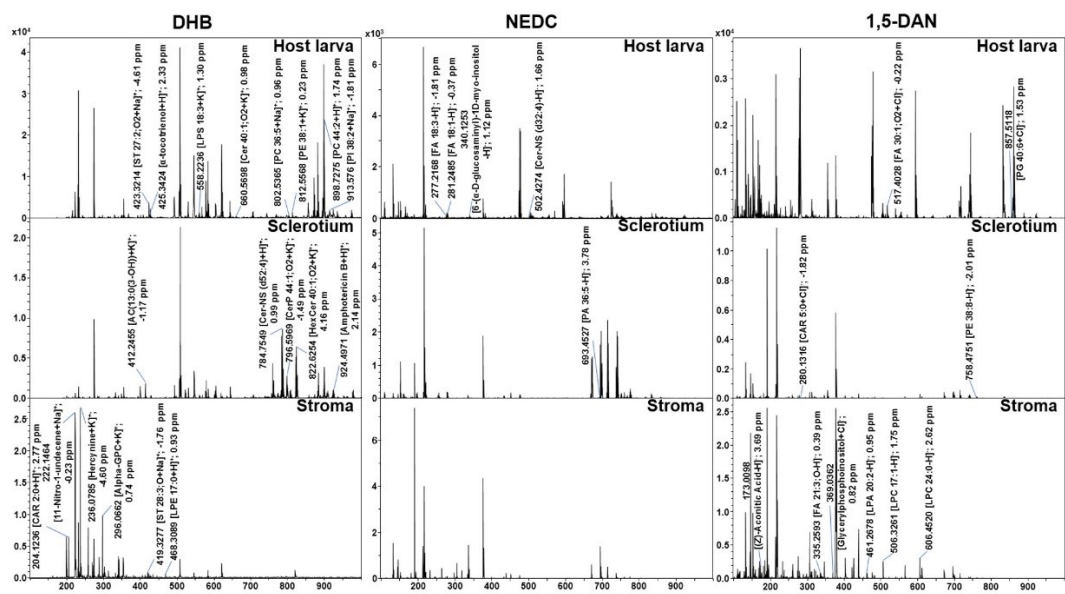


Figure S1. Single-pixel mass spectra with a different matrix. Multiple matrices were used in dual-mode MALDI-MSI to test lipids and other small metabolites. The DHB matrix was used in the positive mode, while NEDC and 1,5-DAN matrices were used in the negative mode.

## Supplementary Table

**Table S1. Compounds putatively identified based on high-resolution MS and MS/MS data.**

Main class	Subclass	Calculated m/z	Measured m/z	Error (ppm)	Ion form	Abbr.	Formula
Fatty Acids and Conjugates [FA01]	Unsaturated fatty acids [FA0103]	277.22	277.22	-1.81	[M-H]-	FA 18:3	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>
Fatty Acids and Conjugates [FA01]	Unsaturated fatty acids [FA0103]	281.25	281.25	-0.37	[M-H]-	FA 18:1	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>
Fatty Acids and Conjugates [FA01]	Hydroxy fatty acids [FA0105]	185.12	185.12	3.68	[M-H]-	FA 10:1;O	C <sub>10</sub> H <sub>18</sub> O <sub>3</sub>
Fatty Acids and Conjugates [FA01]	Heterocyclic fatty acids [FA0115]	335.26	335.26	0.39	[M-H]-	FA 21:3;O	C <sub>21</sub> H <sub>36</sub> O <sub>3</sub>
Fatty Acids and Conjugates [FA01]	Dicarboxylic acids [FA0117]	517.40	517.40	-0.22	[M+Cl]-	FA 30:1;O2	C <sub>30</sub> H <sub>58</sub> O <sub>4</sub>
Eicosanoids [FA03]	Prostaglandins [FA0301]	379.25	379.25	0.27	[M-H]-	FA 22:4;O3	C <sub>22</sub> H <sub>36</sub> O <sub>5</sub>
Eicosanoids [FA03]	Hydroxy/hydroperoxyeicosatetraenoic acids [FA0306]	319.23	319.23	-1.78	[M-H]-	FA 20:4;O	C <sub>20</sub> H <sub>32</sub> O <sub>3</sub>
Fatty esters [FA07]	-	162.11	1162.11	2.46	[M+H]+	Carnitine	C <sub>7</sub> H <sub>15</sub> NO <sub>3</sub>
Fatty esters [FA07]	Fatty acyl carnitines [FA0707]	280.13	280.13	-1.82	[M+Cl]-	CAR 5:0	C <sub>12</sub> H <sub>23</sub> NO <sub>4</sub>
Fatty esters [FA07]	Fatty acyl carnitines [FA0707]	204.12	204.12	2.77	[M+H]+	CAR 2:0	C <sub>9</sub> H <sub>17</sub> NO <sub>4</sub>
Fatty esters [FA07]	Fatty acyl carnitines [FA0707]	254.14	254.14	1.66	[M+Na]+	CAR 4:0	C <sub>11</sub> H <sub>21</sub> NO <sub>4</sub>
Fatty esters [FA07]	Fatty acyl carnitines [FA0707]	238.10	238.11	0.93	[M+Na]+	CAR 3:1	C <sub>10</sub> H <sub>17</sub> NO <sub>4</sub>
Fatty amides [FA08]	N-acyl amines [FA0802]	328.29	328.29	0.86	[M-H]-	NA 19:0;O2	C <sub>19</sub> H <sub>39</sub> NO <sub>3</sub>
Monoradylglycerols [GL01]	Monoacylglycerols [GL0101]	375.25	375.25	0.31	[M-H]-	MG 20:5	C <sub>23</sub> H <sub>36</sub> O <sub>4</sub>
Triradylglycerols [GL03]	Triacylglycerols [GL0301]	835.68	835.68	-2.41	[M-H]-	TG 51:6	C <sub>54</sub> H <sub>92</sub> O <sub>6</sub>
Triradylglycerols [GL03]	Triacylglycerols [GL0301]	871.68	871.68	2.86	[M+Na]+	TG 52:7	C <sub>55</sub> H <sub>92</sub> O <sub>6</sub>
Triradylglycerols [GL03]	Triacylglycerols [GL0301]	879.68	879.68	-0.40	[M+K]+	TG 51:4	C <sub>54</sub> H <sub>96</sub> O <sub>6</sub>
Triradylglycerols [GL03]	Triacylglycerols [GL0301]	895.81	895.81	-3.90	[M+Na]+	TG 54:2	C <sub>57</sub> H <sub>108</sub> O <sub>5</sub>
Triradylglycerols [GL03]	Triacylglycerols [GL0301]	921.79	921.79	-1.91	[M+Na]+	TG 55:3	C <sub>58</sub> H <sub>106</sub> O <sub>6</sub>
Glycerophosphocholines [GP01]	-	296.07	296.07	0.74	[M+K]+	GPC	C <sub>8</sub> H <sub>20</sub> NO <sub>6</sub> P
Glycerophosphocholines [GP01]	Diacylglycerophosphocholines [GP0101]	798.54	798.54	-1.46	[M+K]+	PC 34:1	C <sub>42</sub> H <sub>82</sub> NO <sub>8</sub> P

Glycerophosphocholines [GP01]	Diacylglycerophosphocholines [GP0101]	802.54	802.54	0.96	[M+Na]+	PC 36:5	C <sub>44</sub> H <sub>78</sub> NO <sub>8</sub> P
Glycerophosphocholines [GP01]	Diacylglycerophosphocholines [GP0101]	820.62	820.62	1.27	[M+Na]+	PC O-38:3	C <sub>46</sub> H <sub>88</sub> NO <sub>7</sub> P
Glycerophosphocholines [GP01]	Diacylglycerophosphocholines [GP0101]	898.73	898.73	1.74	[M+H]+	PC 44:2	C <sub>52</sub> H <sub>100</sub> NO <sub>8</sub> P
Glycerophosphocholines [GP01]	1-alkyl,2-acylglycerophosphocholines [GP0102]	556.32	556.32	-4.03	[M+Cl]-	PC O-18:1	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P
Glycerophosphocholines [GP01]	Monoacylglycerophosphocholines [GP0105]	506.33	506.33	1.75	[M-H]-	LPC 17:1	C <sub>25</sub> H <sub>50</sub> NO <sub>7</sub> P
Glycerophosphocholines [GP01]	Monoacylglycerophosphocholines [GP0105]	556.28	556.28	1.98	[M+K]+	LPC 18:3	C <sub>26</sub> H <sub>48</sub> NO <sub>7</sub> P
Glycerophosphocholines [GP01]	Monoacylglycerophosphocholines [GP0105]	606.45	606.45	2.62	[M-H]-	LPC 24:0	C <sub>32</sub> H <sub>66</sub> NO <sub>7</sub> P
Glycerophosphoethanolamines [GP02]	Diacylglycerophosphoethanolamines [GP0201]	714.51	714.51	1.08	[M-H]-	PE 34:2	C <sub>39</sub> H <sub>74</sub> NO <sub>8</sub> P
Glycerophosphoethanolamines [GP02]	Diacylglycerophosphoethanolamines [GP0201]	716.52	716.52	0.17	[M-H]-	PE 34:1	C <sub>39</sub> H <sub>76</sub> NO <sub>8</sub> P
Glycerophosphoethanolamines [GP02]	Diacylglycerophosphoethanolamines [GP0201]	758.48	758.48	-2.01	[M-H]-	PE 38:8	C <sub>43</sub> H <sub>70</sub> NO <sub>8</sub> P
Glycerophosphoethanolamines [GP02]	Diacylglycerophosphoethanolamines [GP0201]	812.56	812.56	0.23	[M+K]+	PE 38:1	C <sub>43</sub> H <sub>84</sub> NO <sub>8</sub> P
Glycerophosphoethanolamines [GP02]	1-alkyl,2-acylglycerophosphoethanolamines [GP0202]	724.53	724.53	-1.05	[M-H]-	PE O-36:4	C <sub>41</sub> H <sub>76</sub> NO <sub>7</sub> P
Glycerophosphoethanolamines [GP02]	1-alkyl,2-acylglycerophosphoethanolamines [GP0202]	726.54	726.54	-1.40	[M-H]-	PE O-36:3	C <sub>41</sub> H <sub>78</sub> NO <sub>7</sub> P
Glycerophosphoethanolamines [GP02]	1-alkyl,2-acylglycerophosphoethanolamines [GP0202]	728.56	728.56	2.38	[M-H]-	PE O-36:2	C <sub>41</sub> H <sub>80</sub> NO <sub>7</sub> P
Glycerophosphoethanolamines [GP02]	1-(1Z-alkenyl),2-acylglycerophosphoethanolamines [GP0203]	738.52	738.52	1.50	[M+Cl]-	PE O-34:1	C <sub>39</sub> H <sub>78</sub> NO <sub>7</sub> P
Glycerophosphoethanolamines [GP02]	Monoacylglycerophosphoethanolamines [GP0205]	452.28	452.28	-3.45	[M-H]-	LPE 16:0	C <sub>21</sub> H <sub>44</sub> NO <sub>7</sub> P
Glycerophosphoethanolamines	Monoacylglycerophosphoethanolamines	468.31	468.31	0.93	[M+H]+	LPE 17:0	C <sub>22</sub> H <sub>46</sub> NO <sub>7</sub> P

[GP02]	[GP0205]							
Glycerophosphoethanolamines [GP02]	Monoacylglycerophosphoethanolamines [GP0205]	474.26	474.26	-0.66	[M-H]-	LPE 18:3	C <sub>23</sub> H <sub>42</sub> NO <sub>7</sub> P	
Glycerophosphoethanolamines [GP02]	Monoacylglycerophosphoethanolamines [GP0205]	476.28	476.28	0.50	[M-H]-	LPE 18:2	C <sub>23</sub> H <sub>44</sub> NO <sub>7</sub> P	
Glycerophosphoethanolamines [GP02]	Monoacylglycerophosphoethanolamines [GP0205]	478.29	478.29	-1.91	[M-H]-	LPE 18:1	C <sub>23</sub> H <sub>46</sub> NO <sub>7</sub> P	
Glycerophosphoethanolamines [GP02]	Monoacylglycerophosphoethanolamines [GP0205]	506.33	506.33	0.37	[M-H]-	LPE 20:1	C <sub>25</sub> H <sub>50</sub> NO <sub>7</sub> P	
Glycerophosphoethanolamines [GP02]	Monoacylglycerophosphoethanolamines [GP0205]	508.34	508.34	4.60	[M-H]-	LPE 20:0	C <sub>25</sub> H <sub>52</sub> NO <sub>7</sub> P	
Glycerophosphoserines [GP03]	Diacylglycerophosphoserines [GP0301]	856.55	856.54	-3.90	[M+K]+	PS 38:1	C <sub>44</sub> H <sub>84</sub> NO <sub>10</sub> P	
Glycerophosphoserines [GP03]	Monoacylglycerophosphoserines [GP0305]	558.22	558.22	1.30	[M+K]+	LPS 18:3	C <sub>24</sub> H <sub>42</sub> NO <sub>9</sub> P	
Glycerophosphoserines [GP03]	Monoacylglycerophosphoserines [GP0305]	562.25	562.26	1.82	[M+K]+	LPS 18:1	C <sub>24</sub> H <sub>46</sub> NO <sub>9</sub> P	
Glycerophosphoglycerols [GP04]	Diacylglycerophosphoglycerols [GP0401]	857.51	857.51	1.53	[M+Cl]-	PG 40:6	C <sub>46</sub> H <sub>79</sub> O <sub>10</sub> P	
Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]	835.53	835.53	-0.12	[M-H]-	PI 34:1	C <sub>43</sub> H <sub>81</sub> O <sub>13</sub> P	
Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]	859.53	859.54	1.86	[M-H]-	PI 36:3	C <sub>45</sub> H <sub>81</sub> O <sub>13</sub> P	
Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]	861.55	861.55	-1.34	[M-H]-	PI 36:2	C <sub>45</sub> H <sub>83</sub> O <sub>13</sub> P	
Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]	863.57	863.57	-0.35	[M-H]-	PI 36:1	C <sub>45</sub> H <sub>85</sub> O <sub>13</sub> P	
Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]	911.56	911.56	-0.66	[M+Na]+	PI 38:3	C <sub>47</sub> H <sub>85</sub> O <sub>13</sub> P	
Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]	913.58	913.58	-1.81	[M+Na]+	PI 38:2	C <sub>47</sub> H <sub>87</sub> O <sub>13</sub> P	
Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]	915.59	915.59	-1.42	[M+Na]+	PI 38:1	C <sub>47</sub> H <sub>89</sub> O <sub>13</sub> P	
Glycerophosphoinositols [GP06]	Diacylglycerophosphoinositols [GP0601]	921.64	921.64	0.27	[M-H]-	PI 40:0	C <sub>49</sub> H <sub>95</sub> O <sub>13</sub> P	
Glycerophosphoinositols [GP06]	Monoacylglycerophosphoinositols [GP0605]	571.29	571.29	0.90	[M-H]-	LPI 16:0	C <sub>25</sub> H <sub>49</sub> O <sub>12</sub> P	
Glycerophosphoinositols [GP06]	Monoacylglycerophosphoinositols [GP0605]	593.27	593.27	1.45	[M-H]-	LPI 18:3	C <sub>27</sub> H <sub>47</sub> O <sub>12</sub> P	
Glycerophosphoinositols [GP06]	Monoacylglycerophosphoinositols [GP0605]	595.29	595.29	-4.35	[M-H]-	LPI 18:2	C <sub>27</sub> H <sub>49</sub> O <sub>12</sub> P	
Glycerophosphoinositols [GP06]	Monoacylglycerophosphoinositols [GP0605]	597.30	597.31	3.29	[M-H]-	LPI 18:1	C <sub>27</sub> H <sub>51</sub> O <sub>12</sub> P	

Glycerophosphates [GP10]	Diacylglycerophosphates [GP1001]	671.47	671.47	2.49	[M-H]-	PA 34:2	C <sub>37</sub> H <sub>69</sub> O <sub>8</sub> P
Glycerophosphates [GP10]	Diacylglycerophosphates [GP1001]	693.45	693.45	3.78	[M-H]-	PA 36:5	C <sub>39</sub> H <sub>67</sub> O <sub>8</sub> P
Glycerophosphates [GP10]	Diacylglycerophosphates [GP1001]	6659.46	659.46	1.51	[M-H]-	PA 33:1	C <sub>36</sub> H <sub>69</sub> O <sub>8</sub> P
Glycerophosphates [GP10]	Diacylglycerophosphates [GP1001]	699.50	699.50	2.39	[M-H]-	PA 36:2	C <sub>39</sub> H <sub>73</sub> O <sub>8</sub> P
Glycerophosphates [GP10]	Monoacylglycerophosphates [GP1005]	461.27	461.27	0.95	[M-H]-	LPA 20:2	C <sub>23</sub> H <sub>43</sub> O <sub>7</sub> P
Glycerophosphates [GP10]	Monoacylglycerophosphates [GP1005]	463.28	463.28	1.05	[M-H]-	LPA 20:1	C <sub>23</sub> H <sub>45</sub> O <sub>7</sub> P
Quinones and hydroquinones [PR02]	Vitamin E [PR0202]	425.34	425.34	2.33	[M+H]+	Tocotrienol	C <sub>29</sub> H <sub>44</sub> O <sub>2</sub>
Sphingoid bases [SP01]	Sphing-4-enines (Sphingosines) [SP0101]	298.28	298.27	-1.18	[M-H]-	SPB 18:1;O2	C <sub>18</sub> H <sub>37</sub> NO <sub>2</sub>
Ceramides [SP02]	N-acylsphingosines (ceramides) [SP0201]	502.43	502.43	1.66	[M-H]-	Cer 32:4;O2	C <sub>32</sub> H <sub>57</sub> NO <sub>3</sub>
Ceramides [SP02]	N-acylsphingosines (ceramides) [SP0201]	544.41	544.41	4.13	[M+K]+	Cer 32:3;O2	C <sub>32</sub> H <sub>59</sub> NO <sub>3</sub>
Ceramides [SP02]	N-acylsphingosines (ceramides) [SP0201]	560.50	560.50	1.40	[M+Na]+	Cer 34:1;O2	C <sub>34</sub> H <sub>67</sub> NO <sub>3</sub>
Ceramides [SP02]	N-acylsphingosines (ceramides) [SP0201]	612.48	612.48	1.87	[M+K]+	Cer 37:4;O2	C <sub>37</sub> H <sub>67</sub> NO <sub>3</sub>
Ceramides [SP02]	N-acylsphingosines (ceramides) [SP0201]	660.57	660.57	0.98	[M+K]+	Cer 40:1;O2	C <sub>40</sub> H <sub>79</sub> NO <sub>3</sub>
Ceramides [SP02]	N-acylsphingosines (ceramides) [SP0201]	784.75	784.75	0.99	[M+H]+	Cer 52:4;O2	C <sub>52</sub> H <sub>97</sub> NO <sub>3</sub>
Ceramides [SP02]	N-acylsphinganine (dihydroceramides) [SP0202]	522.43	522.43	0.76	[M+K]+	Cer 30:0;O2	C <sub>30</sub> H <sub>61</sub> NO <sub>3</sub>
Ceramides [SP02]	N-acyl-4- hydroxysphinganine (phytoceramides) [SP0203]	714.58	714.58	0.31	[M+Cl]-	Cer 42:2;O4	C <sub>42</sub> H <sub>81</sub> NO <sub>5</sub>
Ceramides [SP02]	N-acyl-4- hydroxysphinganine (phytoceramides) [SP0203]	738.70	738.70	-0.27	[M-H]-	Cer 46:0;O4	C <sub>46</sub> H <sub>93</sub> NO <sub>5</sub>
Ceramides [SP02]	Ceramide 1-phosphates [SP0205]	796.60	796.60	-1.49	[M+K]+	CerP 44:1;O2	C <sub>44</sub> H <sub>88</sub> NO <sub>6</sub> P
Neutral glycosphingolipids [SP05]	Simple Glc series [SP0501]	822.62	822.63	4.16	[M+K]+	HexCer 40:1;O2	C <sub>46</sub> H <sub>89</sub> NO <sub>8</sub>
Neutral glycosphingolipids [SP05]	Simple Glc series [SP0501]	882.64	882.65	3.05	[M+K]+	HexCer 42:1;O4	C <sub>48</sub> H <sub>93</sub> NO <sub>10</sub>
Sterols [ST01]	Cholesterol and derivatives [ST0101]	423.32	423.32	-4.61	[M+Na]+	ST 27:2;O2	C <sub>27</sub> H <sub>44</sub> O <sub>2</sub>

	Cholesterol and derivatives [ST0101]	439.36	439.36	-4.45	[M-H]-	ST 30:3;O2	C <sub>30</sub> H <sub>48</sub> O <sub>2</sub>
	Sterol esters [ST0102]	671.58	671.58	-2.17	[M-H]-	CE 20:4	C <sub>47</sub> H <sub>76</sub> O <sub>2</sub>
	Sterol esters [ST0102]	697.59	697.59	0.57	[M-H]-	CE 22:5	C <sub>49</sub> H <sub>78</sub> O <sub>2</sub>
	Ergosterols and C24-methyl derivatives [ST0103]	419.33	419.33	-1.76	[M+Na]+	ST 28:3;O	C <sub>28</sub> H <sub>44</sub> O
Small molecules	Nucleobase	134.05	134.05	4.34	[M-H]-	Adenine	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>
Small molecules	-	135.03	135.03	2.71	[M-H]-	Hypoxanthine	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O
Small molecules	tricarboxylic acid	173.01	173.01	3.69	[M-H]-	Aconitic Acid	C <sub>6</sub> H <sub>6</sub> O <sub>6</sub>
Small molecules	amino acid	145.06	145.06	-4.5	[M-H]-	Glutamine	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Small molecules	sugar alcohol	181.07	181.07	-0.55	[M-H]-	Sorbitol	C <sub>6</sub> H <sub>14</sub> O <sub>6</sub>
Small molecules	nitroalkene	222.15	222.15	-0.23	[M+Na]+	Nitro-undecene	C <sub>11</sub> H <sub>21</sub> NO <sub>2</sub>
Small molecules	amino-acid betaine	236.08	236.08	-4.60	[M+K]+	Hercynine	C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub>
Small molecules	ribonucleoside	268.10	268.10	1.38	[M+H]+	Adenosine	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>
Small molecules	peptide	328.08	328.08	2.90	[M+Cl]-	Glutamyl-Phenylalanine	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O <sub>5</sub>
Small molecules	-	259.12	259.12	-1.54	[M-H]-	Glu-leu	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>
Small molecules	nucleoside	312.13	312.13	3.06	[M+H]+	Dimethylguanosine	C <sub>12</sub> H <sub>17</sub> N <sub>5</sub> O <sub>5</sub>
Small molecules	-	167.02	167.02	4.41	[M-H]-	Uric Acid	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>
Small molecules	-	318.06	318.06	2.30	[M+Cl]-	hydroxy-deoxyguanosine	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>
Small molecules	-	333.07	333.08	1.34	[M+Cl]-	Phenylethanol glucuronide	C <sub>14</sub> H <sub>18</sub> O <sub>7</sub>
Small molecules	-	340.12	340.13	2.30	[M-H]-	glucosaminylmyo-inositol	C <sub>12</sub> H <sub>23</sub> NO <sub>10</sub>
Small molecules	-	369.04	369.04	1.36	[M+Cl]-	Glycerylphosphoinositol	C <sub>9</sub> H <sub>19</sub> O <sub>11</sub> P
Small molecules	-	452.41	452.41	1.29	[M-H]-	Hexacosanoylglycine	C <sub>28</sub> H <sub>55</sub> NO <sub>3</sub>

Note: The compounds were detected by LC-MS and summarized, matching with databases: Lipidmaps and Lipidblast. The lipid categories, including main classes and subclasses, were listed according to the rules of the LIPID MAPS Lipid Classification System.