

# Serum Metabolome Signatures Characterizing Co-Infection of *Plasmodium falciparum* and HBV in Pregnant Women

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## **SUPPLEMENTARY TABLES**

Supplementary Table S1: List of Metabolites Analyzed in the Study

|    | <b>Metabolite</b>      | <b>Full Metabolite Name</b>                         | <b>Metabolite Class</b> |
|----|------------------------|---|-------------------------|
| 1  | <b>C0</b>              | Carnitine   | acylcarnitine           |
| 2  | <b>C2</b>              | Acetylcarnitine                                     | acylcarnitine           |
| 3  | <b>C3</b>              | Propionylcarnitine                                  | acylcarnitine           |
| 4  | <b>C3-DC (C4-OH)</b>   | Hydroxybutyrylcarnitine                             | acylcarnitine           |
| 5  | <b>C3-OH</b>           | Hydroxypropionylcarnitine                           | acylcarnitine           |
| 6  | <b>C3:1</b>            | Propenoylcarnitine                                  | acylcarnitine           |
| 7  | <b>C4</b>              | Butyrylcarnitine                                    | acylcarnitine           |
| 8  | <b>C4:1</b>            | Butenylcarnitine                                    | acylcarnitine           |
| 9  | <b>C5</b>              | Valerylcarnitine                                    | acylcarnitine           |
| 10 | <b>C5-DC (C6-OH)</b>   | Glutarylcarnitine<br>(Hydroxyhexanoylcarnitine)     | acylcarnitine           |
| 11 | <b>C5-M-DC</b>         | Methylglutarylcarnitine                             | acylcarnitine           |
| 12 | <b>C5-OH (C3-DC-M)</b> | Hydroxyvalerylcarnitine<br>(Methylmalonylcarnitine) | acylcarnitine           |

|    |                     |                                       |               |
|----|---------------------|---------------------------------------|---------------|
| 13 | <b>C5:1</b>         | Tiglylcarnitine                       | acylcarnitine |
| 14 | <b>C5:1-DC</b>      | Glutaconylcarnitine                   | acylcarnitine |
| 15 | <b>C6 (C4:1-DC)</b> | Hexanoylcarnitine (Fumaryl carnitine) | acylcarnitine |
| 16 | <b>C6:1</b>         | Hexenoylcarnitine                     | acylcarnitine |
| 17 | <b>C7-DC</b>        | Pimelylcarnitine                      | acylcarnitine |
| 18 | <b>C8</b>           | Octanoylcarnitine                     | acylcarnitine |
| 19 | <b>C9</b>           | Nonaylcarnitine                       | acylcarnitine |
| 20 | <b>C10</b>          | Decanoylcarnitine                     | acylcarnitine |
| 21 | <b>C10:1</b>        | Decenoylcarnitine                     | acylcarnitine |
| 22 | <b>C10:2</b>        | Decadienylcarnitine                   | acylcarnitine |
| 23 | <b>C12</b>          | Dodecanoylcarnitine                   | acylcarnitine |
| 24 | <b>C12-DC</b>       | Dodecenoylcarnitine                   | acylcarnitine |
| 25 | <b>C12:1</b>        | Dodecanedioylcarnitine                | acylcarnitine |
| 26 | <b>C14</b>          | Tetradecanoylcarnitine                | acylcarnitine |
| 27 | <b>C14:1</b>        | Tetradecenoylcarnitine                | acylcarnitine |
| 28 | <b>C14:1-OH</b>     | Hydroxytetradecenoylcarnitine         | acylcarnitine |
| 29 | <b>C14:2</b>        | Tetradecadienylcarnitine              | acylcarnitine |

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|    |                 |                                 |               |
|----|-----------------|---------------------------------|---------------|
| 30 | <b>C14:2-OH</b> | Hydroxytetradecadienylcarnitine | acylcarnitine |
| 31 | <b>C16</b>      | Hexadecanoylcarnitine           | acylcarnitine |
| 32 | <b>C16-OH</b>   | Hexadecenoylcarnitine           | acylcarnitine |
| 33 | <b>C16:1</b>    | Hydroxyhexadecenoylcarnitine    | acylcarnitine |
| 34 | <b>C16:1-OH</b> | Hexadecadienylcarnitine         | acylcarnitine |
| 35 | <b>C16:2</b>    | Hydroxyhexadecadienylcarnitine  | acylcarnitine |
| 36 | <b>C16:2-OH</b> | Hydroxyhexadecanoylcarnitine    | acylcarnitine |
| 37 | <b>C18</b>      | Octadecanoylcarnitine           | acylcarnitine |
| 38 | <b>C18:1</b>    | Octadecenoylcarnitine           | acylcarnitine |
| 39 | <b>C18:1-OH</b> | Hydroxyoctadecenoylcarnitine    | acylcarnitine |
| 40 | <b>C18:2</b>    | Octadecadienylcarnitine         | acylcarnitine |
| 41 | <b>Ala</b>      | Alanine                         | amino acid    |
| 42 | <b>Arg</b>      | Arginine                        | amino acid    |
| 43 | <b>Asn</b>      | Asparagine                      | amino acid    |
| 44 | <b>Asp</b>      | Aspartate                       | amino acid    |
| 45 | <b>Cit</b>      | Citrulline                      | amino acid    |
| 46 | <b>Gln</b>      | Glutamine                       | amino acid    |

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|----|---------------|-----------------------------|----------------|
| 47 | <b>Glu</b>    | Glutamate                   | amino acid     |
| 48 | <b>Gly</b>    | Glycine                     | amino acid     |
| 49 | <b>His</b>    | Histidine                   | amino acid     |
| 50 | <b>Ile</b>    | Isoleucine                  | amino acid     |
| 51 | <b>Leu</b>    | Leucine                     | amino acid     |
| 52 | <b>Lys</b>    | Lysine                      | amino acid     |
| 53 | <b>Met</b>    | Methionine                  | amino acid     |
| 54 | <b>Orn</b>    | Ornithine                   | amino acid     |
| 55 | <b>Phe</b>    | Phenylalanine               | amino acid     |
| 56 | <b>Pro</b>    | Proline                     | amino acid     |
| 57 | <b>Ser</b>    | Serine                      | amino acid     |
| 58 | <b>Thr</b>    | Threonine                   | amino acid     |
| 59 | <b>Trp</b>    | Tryptophan                  | amino acid     |
| 60 | <b>Tyr</b>    | Tyrosine                    | amino acid     |
| 61 | <b>Val</b>    | Valine                      | amino acid     |
| 62 | <b>Ac-Orn</b> | Acetylornithine             | biogenic amine |
| 63 | <b>ADMA</b>   | Asymmetric dimethylarginine | biogenic amine |

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|----|-------------------|----------------------------|----------------|
| 64 | <b>alpha-AAA</b>  | $\alpha$ -Aminoadipic acid | biogenic amine |
| 65 | <b>c4-OH-Pro</b>  | cis-4-Hydroxyproline       | biogenic amine |
| 66 | <b>Carnosine</b>  | Carnosine                  | biogenic amine |
| 67 | <b>Creatinine</b> | Creatinine                 | biogenic amine |
| 68 | <b>DOPA</b>       | Dihydroxyphenylalanine     | biogenic amine |
| 69 | <b>Dopamine</b>   | Dopamine                   | biogenic amine |
| 70 | <b>Histamine</b>  | Histamine                  | biogenic amine |
| 71 | <b>Kynurenine</b> | Kynurenine                 | biogenic amine |
| 72 | <b>Met-SO</b>     | Methionine sulfoxide       | biogenic amine |
| 73 | <b>Nitro-Tyr</b>  | Nitrotyrosine              | biogenic amine |
| 74 | <b>PEA</b>        | Phenylethylamine           | biogenic amine |
| 75 | <b>Putrescine</b> | Putrescine                 | biogenic amine |
| 76 | <b>SDMA</b>       | Symmetric dimethylarginine | biogenic amine |
| 77 | <b>Serotonin</b>  | Serotonin                  | biogenic amine |
| 78 | <b>Spermidine</b> | Spermidine                 | biogenic amine |
| 79 | <b>Spermine</b>   | Spermine                   | biogenic amine |
| 80 | <b>t4-OH-Pro</b>  | trans-4-Hydroxyproline     | biogenic amine |

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|----|-----------------------|------------------------------------|-------------------------|
| 81 | <b>Taurine</b>        | Taurine                            | biogenic amine          |
| 82 | <b>total DMA</b>      | total dimethylarginine             | biogenic amine          |
| 83 | <b>lysoPC a C14:0</b> | lysoPhosphatidylcholine acyl C14:0 | lysophosphatidylcholine |
| 84 | <b>lysoPC a C16:0</b> | lysoPhosphatidylcholine acyl C16:0 | lysophosphatidylcholine |
| 85 | <b>lysoPC a C16:1</b> | lysoPhosphatidylcholine acyl C16:1 | lysophosphatidylcholine |
| 86 | <b>lysoPC a C17:0</b> | lysoPhosphatidylcholine acyl C17:0 | lysophosphatidylcholine |
| 87 | <b>lysoPC a C18:0</b> | lysoPhosphatidylcholine acyl C18:0 | lysophosphatidylcholine |
| 88 | <b>lysoPC a C18:1</b> | lysoPhosphatidylcholine acyl C18:1 | lysophosphatidylcholine |
| 89 | <b>lysoPC a C18:2</b> | lysoPhosphatidylcholine acyl C18:2 | lysophosphatidylcholine |
| 90 | <b>lysoPC a C20:3</b> | lysoPhosphatidylcholine acyl C20:3 | lysophosphatidylcholine |
| 91 | <b>lysoPC a C20:4</b> | lysoPhosphatidylcholine acyl C20:4 | lysophosphatidylcholine |
| 92 | <b>lysoPC a C24:0</b> | lysoPhosphatidylcholine acyl C24:0 | lysophosphatidylcholine |
| 93 | <b>lysoPC a C26:0</b> | lysoPhosphatidylcholine acyl C26:0 | lysophosphatidylcholine |
| 94 | <b>lysoPC a C26:1</b> | lysoPhosphatidylcholine acyl C26:1 | lysophosphatidylcholine |
| 95 | <b>lysoPC a C28:0</b> | lysoPhosphatidylcholine acyl C28:0 | lysophosphatidylcholine |
| 96 | <b>lysoPC a C28:1</b> | lysoPhosphatidylcholine acyl C28:1 | lysophosphatidylcholine |
| 97 | <b>PC aa C24:0</b>    | Phosphatidylcholine diacyl C24:0   | phosphatidylcholine     |

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| 98  | <b>PC aa C26:0</b> | Phosphatidylcholine diacyl C26:0 | phosphatidylcholine |
| 99  | <b>PC aa C28:1</b> | Phosphatidylcholine diacyl C28:1 | phosphatidylcholine |
| 100 | <b>PC aa C30:0</b> | Phosphatidylcholine diacyl C30:0 | phosphatidylcholine |
| 101 | <b>PC aa C30:2</b> | Phosphatidylcholine diacyl C30:2 | phosphatidylcholine |
| 102 | <b>PC aa C32:0</b> | Phosphatidylcholine diacyl C32:0 | phosphatidylcholine |
| 103 | <b>PC aa C32:1</b> | Phosphatidylcholine diacyl C32:1 | phosphatidylcholine |
| 104 | <b>PC aa C32:2</b> | Phosphatidylcholine diacyl C32:2 | phosphatidylcholine |
| 105 | <b>PC aa C32:3</b> | Phosphatidylcholine diacyl C32:3 | phosphatidylcholine |
| 106 | <b>PC aa C34:1</b> | Phosphatidylcholine diacyl C34:1 | phosphatidylcholine |
| 107 | <b>PC aa C34:2</b> | Phosphatidylcholine diacyl C34:2 | phosphatidylcholine |
| 108 | <b>PC aa C34:3</b> | Phosphatidylcholine diacyl C34:3 | phosphatidylcholine |
| 109 | <b>PC aa C34:4</b> | Phosphatidylcholine diacyl C34:4 | phosphatidylcholine |
| 110 | <b>PC aa C36:0</b> | Phosphatidylcholine diacyl C36:0 | phosphatidylcholine |
| 111 | <b>PC aa C36:1</b> | Phosphatidylcholine diacyl C36:1 | phosphatidylcholine |
| 112 | <b>PC aa C36:2</b> | Phosphatidylcholine diacyl C36:2 | phosphatidylcholine |
| 113 | <b>PC aa C36:3</b> | Phosphatidylcholine diacyl C36:3 | phosphatidylcholine |
| 114 | <b>PC aa C36:4</b> | Phosphatidylcholine diacyl C36:4 | phosphatidylcholine |

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| 115 | <b>PC aa C36:5</b> | Phosphatidylcholine diacyl C36:5 | phosphatidylcholine |
| 116 | <b>PC aa C36:6</b> | Phosphatidylcholine diacyl C36:6 | phosphatidylcholine |
| 117 | <b>PC aa C38:0</b> | Phosphatidylcholine diacyl C38:0 | phosphatidylcholine |
| 118 | <b>PC aa C38:1</b> | Phosphatidylcholine diacyl C38:1 | phosphatidylcholine |
| 119 | <b>PC aa C38:3</b> | Phosphatidylcholine diacyl C38:3 | phosphatidylcholine |
| 120 | <b>PC aa C38:4</b> | Phosphatidylcholine diacyl C38:4 | phosphatidylcholine |
| 121 | <b>PC aa C38:5</b> | Phosphatidylcholine diacyl C38:5 | phosphatidylcholine |
| 122 | <b>PC aa C38:6</b> | Phosphatidylcholine diacyl C38:6 | phosphatidylcholine |
| 123 | <b>PC aa C40:1</b> | Phosphatidylcholine diacyl C40:1 | phosphatidylcholine |
| 124 | <b>PC aa C40:2</b> | Phosphatidylcholine diacyl C40:2 | phosphatidylcholine |
| 125 | <b>PC aa C40:3</b> | Phosphatidylcholine diacyl C40:3 | phosphatidylcholine |
| 126 | <b>PC aa C40:4</b> | Phosphatidylcholine diacyl C40:4 | phosphatidylcholine |
| 127 | <b>PC aa C40:5</b> | Phosphatidylcholine diacyl C40:5 | phosphatidylcholine |
| 128 | <b>PC aa C40:6</b> | Phosphatidylcholine diacyl C40:6 | phosphatidylcholine |
| 129 | <b>PC aa C42:0</b> | Phosphatidylcholine diacyl C42:0 | phosphatidylcholine |
| 130 | <b>PC aa C42:1</b> | Phosphatidylcholine diacyl C42:1 | phosphatidylcholine |
| 131 | <b>PC aa C42:2</b> | Phosphatidylcholine diacyl C42:2 | phosphatidylcholine |

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| 132 | <b>PC aa C42:4</b> | Phosphatidylcholine diacyl C42:4     | phosphatidylcholine |
| 133 | <b>PC aa C42:5</b> | Phosphatidylcholine diacyl C42:5     | phosphatidylcholine |
| 134 | <b>PC aa C42:6</b> | Phosphatidylcholine diacyl C42:6     | phosphatidylcholine |
| 135 | <b>PC ae C30:0</b> | Phosphatidylcholine acyl-alkyl C30:0 | phosphatidylcholine |
| 136 | <b>PC ae C30:1</b> | Phosphatidylcholine acyl-alkyl C30:1 | phosphatidylcholine |
| 137 | <b>PC ae C30:2</b> | Phosphatidylcholine acyl-alkyl C30:2 | phosphatidylcholine |
| 138 | <b>PC ae C32:1</b> | Phosphatidylcholine acyl-alkyl C32:1 | phosphatidylcholine |
| 139 | <b>PC ae C32:2</b> | Phosphatidylcholine acyl-alkyl C32:2 | phosphatidylcholine |
| 140 | <b>PC ae C34:0</b> | Phosphatidylcholine acyl-alkyl C34:0 | phosphatidylcholine |
| 141 | <b>PC ae C34:1</b> | Phosphatidylcholine acyl-alkyl C34:1 | phosphatidylcholine |
| 142 | <b>PC ae C34:2</b> | Phosphatidylcholine acyl-alkyl C34:2 | phosphatidylcholine |
| 143 | <b>PC ae C34:3</b> | Phosphatidylcholine acyl-alkyl C34:3 | phosphatidylcholine |
| 144 | <b>PC ae C36:0</b> | Phosphatidylcholine acyl-alkyl C36:0 | phosphatidylcholine |
| 145 | <b>PC ae C36:1</b> | Phosphatidylcholine acyl-alkyl C36:1 | phosphatidylcholine |
| 146 | <b>PC ae C36:2</b> | Phosphatidylcholine acyl-alkyl C36:2 | phosphatidylcholine |
| 147 | <b>PC ae C36:3</b> | Phosphatidylcholine acyl-alkyl C36:3 | phosphatidylcholine |
| 148 | <b>PC ae C36:4</b> | Phosphatidylcholine acyl-alkyl C36:4 | phosphatidylcholine |

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| 149 | <b>PC ae C36:5</b>  | Phosphatidylcholine acyl-alkyl C36:5 | phosphatidylcholine |
| 150 | <b>PC ae C38:0</b>  | Phosphatidylcholine acyl-alkyl C38:0 | phosphatidylcholine |
| 151 | <b>PC ae C38:1</b>  | Phosphatidylcholine acyl-alkyl C38:1 | phosphatidylcholine |
| 152 | <b>PC ae C38:2</b>  | Phosphatidylcholine acyl-alkyl C38:2 | phosphatidylcholine |
| 153 | <b>PC ae C38:3</b>  | Phosphatidylcholine acyl-alkyl C38:3 | phosphatidylcholine |
| 154 | <b>PC ae C38:4</b>  | Phosphatidylcholine acyl-alkyl C38:4 | phosphatidylcholine |
| 155 | <b>PC ae C38:5</b>  | Phosphatidylcholine acyl-alkyl C38:5 | phosphatidylcholine |
| 156 | <b>PC ae C38:6</b>  | Phosphatidylcholine acyl-alkyl C38:6 | phosphatidylcholine |
| 157 | <b>PC ae C40:1</b>  | Phosphatidylcholine acyl-alkyl C40:1 | Phosphatidylcholine |
| 158 | <b>PC ae C40:2</b>  | Phosphatidylcholine acyl-alkyl C40:2 | phosphatidylcholine |
| 159 | <b>PC ae C40:3</b>  | Phosphatidylcholine acyl-alkyl C40:3 | phosphatidylcholine |
| 160 | <b>PC ae C40:4</b>  | Phosphatidylcholine acyl-alkyl C40:4 | phosphatidylcholine |
| 161 | <b>PC ae C40:5</b>  | Phosphatidylcholine acyl-alkyl C40:5 | phosphatidylcholine |
| 162 | <b>PC ae C40:6</b>  | Phosphatidylcholine acyl-alkyl C40:6 | phosphatidylcholine |
| 163 | <b>PC ae C42:0</b>  | Phosphatidylcholine acyl-alkyl C42:0 | phosphatidylcholine |
| 164 | <b>PC \ae C42:1</b> | Phosphatidylcholine acyl-alkyl C42:1 | phosphatidylcholine |
| 165 | <b>PC ae C42:2</b>  | Phosphatidylcholine acyl-alkyl C42:2 | phosphatidylcholine |

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|     |                      |                                      |                     |
|-----|----------------------|--------------------------------------|---------------------|
| 166 | <b>PC ae C42:3</b>   | Phosphatidylcholine acyl-alkyl C42:3 | phosphatidylcholine |
| 167 | <b>PC ae C42:4</b>   | Phosphatidylcholine acyl-alkyl C42:4 | phosphatidylcholine |
| 168 | <b>PC ae C42:5</b>   | Phosphatidylcholine acyl-alkyl C42:5 | phosphatidylcholine |
| 169 | <b>PC ae C44:3</b>   | Phosphatidylcholine acyl-alkyl C44:3 | phosphatidylcholine |
| 170 | <b>PC ae C44:4</b>   | Phosphatidylcholine acyl-alkyl C44:4 | phosphatidylcholine |
| 171 | <b>PC ae C44:5</b>   | Phosphatidylcholine acyl-alkyl C44:5 | phosphatidylcholine |
| 172 | <b>PC ae C44:6</b>   | Phosphatidylcholine acyl-alkyl C44:6 | phosphatidylcholine |
| 173 | <b>SM (OH) C14:1</b> | Hydroxysphingomyeline C14:1          | sphingolipid        |
| 174 | <b>SM (OH) C16:1</b> | Hydroxysphingomyeline C16:1          | sphingolipid        |
| 175 | <b>SM (OH) C22:1</b> | Hydroxysphingomyeline C22:1          | sphingolipid        |
| 176 | <b>SM (OH) C22:2</b> | Hydroxysphingomyeline C22:2          | sphingolipid        |
| 177 | <b>SM (OH) C24:1</b> | Hydroxysphingomyeline C24:1          | sphingolipid        |
| 178 | <b>SM C16:0</b>      | Sphingomyeline C16:0                 | sphingolipid        |

|     |                 |                              |              |
|-----|-----------------|------------------------------|--------------|
| 179 | <b>SM C16:1</b> | Sphingomyeline C16:1         | sphingolipid |
| 180 | <b>SM C18:0</b> | Sphingomyeline C18:0         | sphingolipid |
| 181 | <b>SM C18:1</b> | Sphingomyeline C18:1         | sphingolipid |
| 182 | <b>SM C20:2</b> | Sphingomyeline C20:2         | sphingolipid |
| 183 | <b>SM C22:3</b> | Sphingomyeline C22:3         | sphingolipid |
| 184 | <b>SM C24:0</b> | Sphingomyeline C24:0         | sphingolipid |
| 185 | <b>SM C24:1</b> | Sphingomyeline C24:1         | sphingolipid |
| 186 | <b>SM C26:0</b> | Sphingomyeline C26:0         | sphingolipid |
| 187 | <b>SM C26:1</b> | Sphingomyeline C26:1         | sphingolipid |
| 188 | <b>H1</b>       | Sum of Hexoses (90% glucose) | sugar        |

Supplementary Table S2: Demographics of archival samples

| Sample group                      | Mean age/years | Primigravida/% | Multigravida/% | 1 <sup>st</sup> trimester | 2 <sup>nd</sup> trimester | 3 <sup>rd</sup> trimester |
|-----------------------------------|----------------|----------------|----------------|---------------------------|---------------------------|---------------------------|
| Malaria only                      | 25.5           | 32.5           | 67.5           | 30                        | 57.5                      | 12.5                      |
| CHB only                          | 26.7           | 23.5           | 76.5           | 45.6                      | 47.1                      | 7.4                       |
| Malaria+CHB                       | 26.9           | 25             | 75             | 33.3                      | 58.3                      | 8.3                       |
| Uninfected                        | 27.6           | 16.4           | 83.3           | 35.6                      | 46.6                      | 17.8                      |
| P-value (95% confidence interval) | 0.099          | 0.1466         |                | 0.257                     |                           |                           |

Supplementary Table S3: Table Venn diagram results showing the metabolite elements shared among the disease groups

| Comparison groups             | Total metabolites altered | Metabolite elements   |
|-------------------------------|---------------------------|---|
| Co-infected & Hep B & Malaria | 13                        | PC ae C44:4 SM (OH) C22:1 SM C16:0 SM C22:3 SM (OH) C16:1 SM (OH) C14:1 PC aa C28:1 PC aa C40:5 SM C16:1 SM C24:0 SM (OH) C22:2 PC aa C38:5 SM C24:1  |
| Hep B & Malaria               | 1                         | PC aa C32:0   |
| Co-infected & Malaria         | 4                         | PC aa C38:6 SM C18:0 SM (OH) C24:1 SM C18:1   |
| Co-infected & Hep B           | 52                        | PC ae C42:2 PC ae C40:1 PC ae C42:3 PC aa C32:3 PC aa C34:4 PC ae C42:5 PC ae C36:2 PC ae C36:5 Trp PC aa C36:4 PC ae C30:2 PC aa C40:1 PC aa C42:4 PC ae C42:4 PC aa C40:3 PC aa C26:0 PC aa C40:2 PC aa C38:1 PC aa C24:0 PC aa C34:3 PC aa C36:3 PC aa C32:2 PC ae C44:6 PC ae C36:3 PC aa C34:1 lysoPC a C26:1 PC ae C38:4 PC ae C34:3 PC ae C40:6 PC aa C38:3 PC ae C40:3 H1 PC ae C38:3 PC ae C34:2 PC ae C44:5 PC aa C40:4 PC ae C38:2 PC ae C40:4 PC aa C36:2 PC aa C42:5 PC ae C40:2 PC aa C42:6 PC ae C42:1 PC aa C42:1 PC ae C38:1 PC aa C42:2 PC ae C36:1 PC aa C36:1 PC ae C42:0 PC ae C40:5 PC aa C34:2 PC aa C38:4 |
| Malaria                       | 4                         | C14:1 Lys Thr C16:1-OH Asp Phe PC aa C42:0 PC ae C38:5 lysoPC a C24:0 Kynurenine lysoPC a C18:0 lysoPC a C28:0 PC aa C30:0 PC ae C36:4 C4 PC ae C34:0 Pro C4:1  |
| Hep B                         | 18                        | Serotonin Arg C6:1 PC ae C30:1 C5-OH (C3-DC-M) PC aa C40:6 PC aa C36:6 SM C20:2 PC aa C36:5 PC aa C36:0 PC ae C44:3 C5-M-DC PC aa C38:0 PC ae C38:0 Val PC ae C38:6 PC ae C32:2   |
| Co-infected                   | 13                        |   |

Supplementary Table S4: Area Under the Curve (AUC) values for univariate biomarker analysis in the malaria vs uninfected groups

| Biomarker                    | AUC      | P-value from<br>T-test | Log 2 Fold<br>Change | Cluster |
|------------------------------|----------|------------------------|----------------------|---------|
| PC aa C28:1/PC aa C32:0      | 0.756031 | 9.52E-07               | 0.16535              | 2       |
| PC aa C32:0/SM (OH)<br>C22:2 | 0.742599 | 0.000355               | 0.95456              | 5       |
| C16:1-OH/SM (OH)<br>C22:2    | 0.739583 | 0.000612               | -0.09203             | 3       |
| PC aa C32:0/PC ae C44:4      | 0.735197 | 4.32E-05               | 0.11374              | 5       |
| PC aa C32:0/SM (OH)<br>C16:1 | 0.724507 | 0.000618               | 0.24042              | 5       |
| PC aa C32:0/PC aa C38:5      | 0.723684 | 2.41E-05               | -0.61225             | 5       |
| PC aa C32:0/SM (OH)<br>C14:1 | 0.723684 | 0.000617               | 0.32978              | 5       |
| Lys/PC aa C32:0              | 0.71875  | 1.17E-05               | -0.12705             | 2       |
| C16:1-OH/PC aa C38:5         | 0.715186 | 0.000121               | -0.06976             | 3       |
| C16:1-OH/SM C22:3            | 0.715186 | 4.53E-05               | -0.35812             | 3       |
| C16:1-OH/PC aa C28:1         | 0.709978 | 5.20E-05               | -0.11246             | 3       |
| C16:1-OH/Lys                 | 0.706826 | 4.92E-05               | -0.04493             | 3       |
| C16:1-OH/SM (OH)<br>C16:1    | 0.705866 | 0.000645               | -0.1053              | 3       |
| C16:1-OH/PC aa C40:5         | 0.703673 | 0.000454               | -0.07683             | 3       |
| PC aa C32:0/PC aa C40:5      | 0.70148  | 6.75E-05               | 0.92344              | 5       |

AUC cutoff >0.7



Supplementary Table S5: Area Under the Curve (AUC) values for univariate biomarker analysis in the Hepatitis B vs uninfected groups

| Biomarker   | AUC      | P-value from<br>T-test | Log 2 Fold<br>Change | Cluster |
|-------------|----------|------------------------|----------------------|---------|
| Asp         | 0.748736 | 5.29E-06               | -0.67548             | 4       |
| Phe         | 0.73966  | 0.008831               | -0.20458             | 4       |
| PC aa C36:2 | 0.727252 | 3.33E-05               | -0.32898             | 2       |
| SM C24:0    | 0.723346 | 4.57E-06               | -0.31286             | 2       |
| PC aa C40:1 | 0.715188 | 0.000282               | -0.35356             | 5       |
| PC aa C40:4 | 0.709674 | 2.37E-05               | -0.38036             | 2       |
| PC ae C44:4 | 0.70795  | 3.24E-05               | -0.38927             | 2       |
| PC aa C38:4 | 0.705193 | 2.92E-05               | -0.36599             | 3       |
| PC ae C42:4 | 0.704159 | 3.31E-05               | -0.3797              | 2       |

AUC cutoff >0.7

Supplementary Table S6: Area Under the Curve (AUC) values for univariate biomarker analysis in the Co-infected vs uninfected groups

| Biomarker               | AUC      | P-value from<br>T-test | Log 2 Fold<br>Change | Cluster |
|-------------------------|----------|------------------------|----------------------|---------|
| PC ae C40:1             | 0.801649 | 5.91E-05               | -99                  | 2       |
| PC ae C42:3             | 0.792318 | 1.65E-05               | 1.7544               | 2       |
| PC aa C42:5             | 0.785807 | 0.000568               | 0.47364              | 2       |
| SM C24:1                | 0.777778 | 1.97E-06               | -0.09774             | 5       |
| SM (OH) C22:2           | 0.776259 | 2.16E-06               | -0.32341             | 5       |
| PC ae C42:5             | 0.775608 | 0.000245               | -0.5096              | 2       |
| PC aa C40:1             | 0.770833 | 0.003732               | 0.47242              | 2       |
| PC aa C28:1             | 0.767578 | 3.34E-05               | 1.6285               | 1       |
| SM C24:0                | 0.766927 | 6.06E-06               | -0.12553             | 5       |
| PC aa C32:3             | 0.759766 | 0.002364               | 0.26904              | 2       |
| PC ae C42:4             | 0.756944 | 0.003386               | -1.8317              | 2       |
| PC ae C42:2             | 0.754123 | 0.004381               | 0.48377              | 2       |
| PC ae C42:3/PC ae C34:2 | 0.748698 | 2.84E-05               | 0.18265              | 3       |
| PC aa C42:6             | 0.74783  | 0.000665               | 0.58209              | 4       |
| SM (OH) C24:1           | 0.746962 | 0.000192               | 0.92823              | 5       |
| PC aa C40:4             | 0.746962 | 0.000406               | -0.36234             | 4       |
| PC aa C42:1             | 0.746745 | 0.000908               | 0.28211              | 4       |
| SM (OH) C22:1           | 0.744575 | 0.000942               | -0.17261             | 5       |
| SM (OH) C22:1.1         | 0.744575 | 0.000942               | -0.17261             | 5       |
| PC aa C40:3             | 0.743273 | 0.001578               | 1.3363               | 2       |
| PC ae C40:6             | 0.742405 | 0.001496               | -0.39989             | 4       |
| SM C16:0                | 0.742405 | 0.001702               | -0.06236             | 5       |
| PC aa C42:4             | 0.738498 | 0.018837               | 0.59855              | 2       |
| PC ae C40:4             | 0.73763  | 0.006181               | -0.36582             | 2       |
| PC ae C40:1/PC aa C36:1 | 0.737413 | 0.001521               | 0.096368             | 3       |
| PC ae C40:5             | 0.736545 | 0.002143               | -0.30212             | 2       |
| PC aa C24:0             | 0.735677 | 0.000111               | 0.41141              | 1       |
| PC ae C42:0             | 0.735026 | 0.006807               | 0.48461              | 4       |
| PC ae C42:3/PC aa C36:1 | 0.734809 | 0.000214               | 0.10182              | 3       |
| PC ae C40:1/PC ae C34:2 | 0.733507 | 0.0003                 | 0.18636              | 3       |
| SM C20:2                | 0.728733 | 0.001923               | 0.25816              | 5       |
| PC ae C42:3/PC ae C36:3 | 0.727865 | 0.000161               | 0.23139              | 3       |
| PC ae C40:2             | 0.726563 | 0.026784               | -1.9027              | 2       |
| SM (OH) C14:1           | 0.723741 | 0.000128               | -0.39355             | 5       |
| PC ae C40:1/PC aa C36:2 | 0.721354 | 0.000488               | 0.074368             | 3       |
| PC ae C40:1/PC ae C36:3 | 0.72092  | 0.001116               | 0.24842              | 3       |
| SM C18:0                | 0.720486 | 0.000168               | -0.14951             | 5       |
| PC aa C38:1             | 0.720269 | 0.006709               | 1.1939               | 2       |

| Biomarker               | AUC      | P-value from<br>T-test | Log 2 Fold<br>Change | Cluster |
|-------------------------|----------|------------------------|----------------------|---------|
| PC ae C42:3/PC aa C36:2 | 0.720052 | 0.000137               | 0.079704             | 3       |
| PC aa C36:6             | 0.71875  | 0.001209               | 0.86211              | 2       |
| SM (OH) C16:1           | 0.717231 | 9.61E-05               | -0.94976             | 5       |
| PC ae C42:3/PC aa C38:0 | 0.716146 | 0.000274               | 0.3782               | 3       |
| PC aa C36:0             | 0.71441  | 0.165218               | -0.5834              | 2       |
| SM C16:1                | 0.71224  | 0.010459               | -0.13557             | 5       |
| PC aa C38:5             | 0.712023 | 0.001268               | -0.12753             | 4       |
| PC ae C44:4             | 0.711806 | 0.01122                | 0.24332              | 4       |
| PC ae C42:3/PC ae C32:2 | 0.711372 | 0.000146               | -0.47905             | 3       |
| PC aa C38:3             | 0.709201 | 0.016079               | -0.0896              | 4       |
| PC ae C42:3/PC aa C34:1 | 0.709201 | 0.000127               | 0.06871              | 3       |
| PC aa C34:3             | 0.70855  | 0.001508               | -0.30132             | 2       |
| PC ae C38:4             | 0.705512 | 0.025892               | -0.15552             | 4       |
| PC ae C36:1             | 0.702691 | 0.003868               | -0.23862             | 2       |
| PC ae C42:3/PC ae C38:6 | 0.702691 | 0.00054                | 0.23177              | 3       |
| PC ae C42:1             | 0.702257 | 0.004484               | 0.44241              | 2       |
| PC aa C36:3             | 0.702257 | 0.008219               | -0.06669             | 4       |
| PC ae C38:0             | 0.700087 | 0.006332               | -0.64977             | 2       |

AUC cutoff >0.7