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Survival of the littlest: improving preterm outcomes through metabolomics and microsampling

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CHAPTER III

Survival of the Littlest: Navigating Sepsis Diagnosis beyond Inflammation in Preterm Neonates

Based on:

Survival of the littlest: Navigating sepsis diagnosis beyond inflammation in preterm neonates

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Abstract

Sepsis diagnosis in preterm neonates is challenging due to symptom overlap with non-infectious inflammatory conditions, and slow, unreliable diagnostic practices. This case-control study aims to elucidate sepsis pathophysiology, and identify metabolic biomarkers for timely, accurate diagnosis, to prevent rapid health deterioration and unnecessary antibiotic use. Liquid chromatography-mass spectrometry was performed on 227 plasma samples, obtained from 94 preterm neonates, to measure 317 metabolites encompassing amines and signaling lipids. Linear mixed-effect modeling, LASSO and logistic regression models were calculated to assess metabolic alterations across control, systemic inflammation-no sepsis (SINS), and sepsis groups. Stratification by sex and pathogen type allowed identification of sex-specific responses and pathogen-driven variations in sepsis. Key findings include (i) shared metabolic changes in SINS and sepsis, (ii) progressive alterations from control to SINS to sepsis, and (iii) sepsis-specific markers. Males exhibited a pro-inflammatory phenotype while females showed an anti-inflammatory phenotype in response to sepsis. Gram-positive and gram-negative bacterial sepsis revealed distinct metabolic profiles. A diagnostic model comprising 5 metabolic features and IL-6 distinguished SINS from sepsis at clinical suspicion (AUC 0.79, sensitivity 0.85, specificity 0.82). These insights highlight the potential of metabolomics to revolutionize neonatal sepsis management with precision diagnostics and personalized treatment strategies.

1. Introduction

Preterm birth, defined as delivery before 37 weeks of gestation, accounts for approximately 1 in 10 live births globally.¹ While advancements in antenatal care have not significantly reduced the global preterm birth rate, postnatal care interventions have increased the survival probability of even the extremely preterm neonates (<28 weeks gestational age).^{1,2} However, complications associated with prematurity remain the leading cause of adverse health outcomes and under-five mortality.^{3,4} A major contributor to neonatal mortality and long-term morbidity is neonatal sepsis, a systemic infection of microbial origin that occurs within the first month of life.⁵ Neonatal sepsis affects an estimated 1.3 million neonates annually worldwide resulting in ~203,000 deaths, with higher incidence and mortality rates in males compared to females.^{5,6} Time of onset classifies neonatal sepsis as early-onset sepsis, occurring within 72 hours of life typically from bacterial infections vertically transmitted during birth, or late-onset sepsis (LOS) which develops after 72 hours from postnatal environmental exposures.⁵ Early-onset sepsis incidence has declined over the years due to advanced screening and intrapartum antibiotic prophylaxis, but LOS rates have remained unchanged, posing a persistent burden to neonatal healthcare.⁵

The third international consensus defines sepsis as a life-threatening organ dysfunction caused by a dysregulated host response to an infection, providing a valuable diagnostic framework for adults.⁷ However, neonatal sepsis presents with a multitude of inconclusive symptoms, such as abnormal vital signs and feeding intolerance, and gestational- and postnatal-age-dependent variability in clinical presentations, which necessitates a comprehensive approach incorporating various clinical criteria, laboratory markers, and microbiological data (**Figure 1a**).^{5,8} Although blood cultures are the golden standard for sepsis confirmation, their turnover time of ~48h precludes timely interventions, and non-culturable or insufficient live pathogens in samples return false culture-negative results.⁵ Inflammatory biomarkers such as c-reactive protein (CRP), interleukin-6 (IL-6), and procalcitonin (PCT), offer a robust negative predictive value to rule out infections but lack sensitivity and specificity to accurately distinguish sepsis from other non-infectious inflammatory conditions.⁵ Compounding the challenge, sepsis caused by gram-negative bacteria often presents with more severe symptoms and higher mortality than gram-positive bacteria, compelling the empirical use of broad-spectrum antibiotics to all neonates upon sepsis suspicion (**Figure 1a**).^{5,9} However, this practice risks unnecessary antibiotic use, contributing to multidrug-resistant pathogens and gut microbiome disruption which may result in long-term conditions like obesity and asthma.¹⁰ Therefore, early identification of causative pathogens is crucial for tailoring antibiotic therapy and mitigating these risks.

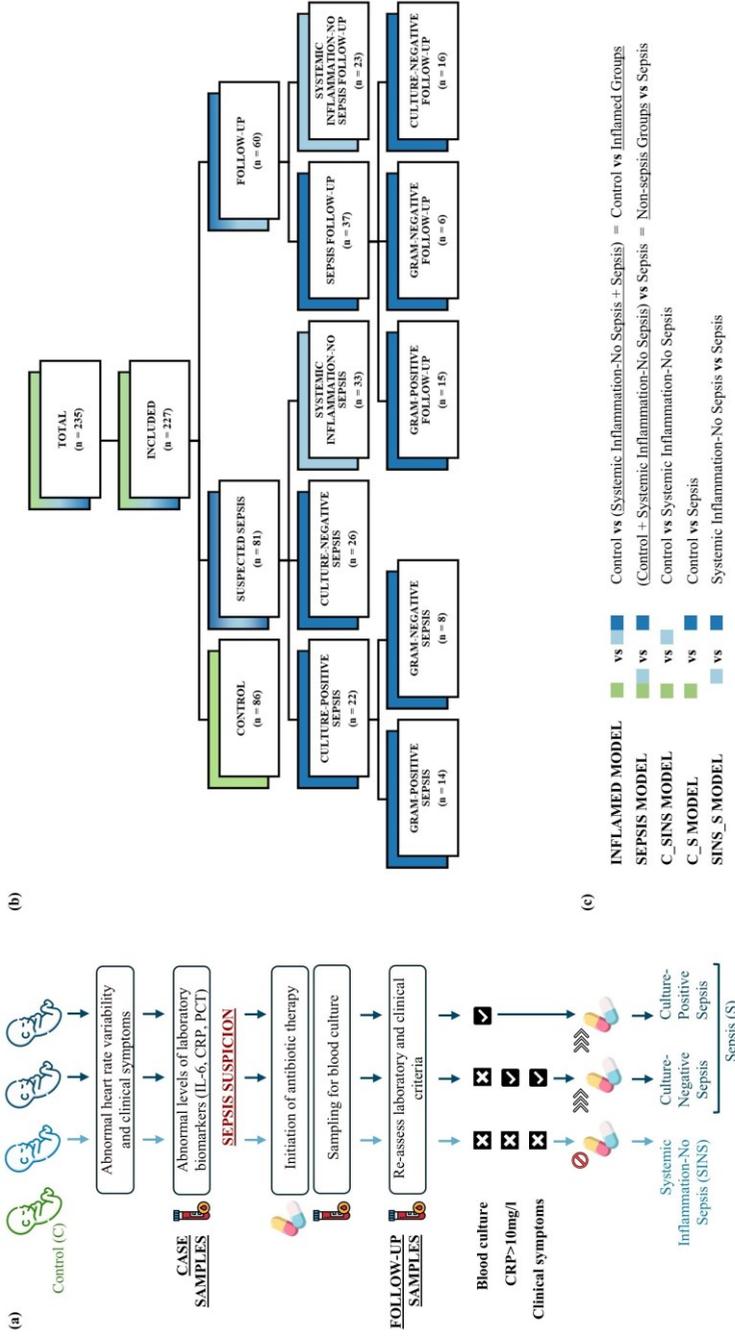


Figure 1. Overview of sample classification criteria, cohort composition, and metabolic modeling framework. (a) The flowchart illustrates the clinical trajectories and criteria for classifying neonates into control, systemic inflammation-no sepsis, culture-negative sepsis and culture-positive sepsis groups, based on clinical symptoms, laboratory findings, and microbiological results. (b) The flowchart depicts the cohort composition, with samples initially classified into control, suspected sepsis, and follow-up samples. For statistical analyses, all samples were grouped into three distinct categories: control (*green*; n=86), systemic inflammation-no sepsis (*light blue*; n=56), and sepsis (*blue*; n=85), wherein the follow-up samples were re-classified into either sepsis or systemic inflammation-no sepsis based on their initial diagnosis. (c) The primary models compared Control vs Inflamed groups and Non-Sepsis groups vs Sepsis to identify systemic inflammation- and sepsis-specific traits. Additional pairwise comparisons were performed between groups: Control vs. Systemic Inflammation-No Sepsis (C_SINS), Control vs. Sepsis (C_S), and Systemic Inflammation-No Sepsis vs. Sepsis (SINS_S). IL-6 = Interleukin-6; CRP = C-Reactive Protein; PCT = Procalcitonin. Icons used in the figure are from Flaticon. (www.flaticon.com)

Metabolomics offers a promising avenue to elucidate sepsis pathophysiology and discover novel biomarkers to complement traditional diagnostic methods. Metabolism plays a vital role in immune cell differentiation and function, influencing both the effector and resolution phases of inflammation. Key pathways, including glycolysis, oxidative phosphorylation, fatty acid (FA) oxidation, and amino acid metabolism, have been implicated in immune regulation.¹¹ The reconfiguration of immunometabolism during inflammatory disorders thus provides insights into disease mechanisms and outcomes. Metabolomic studies investigating LOS in preterm neonates are scarce but have unveiled significant disruptions of biological pathways and imbalances in biochemical homeostasis.^{12–16} However, these studies often compare sepsis cases with controls showing no signs of sepsis or lack clear specification of the inclusion/exclusion criteria for the groups under comparison. This methodological limitation overlooks the critical aspect of identifying sepsis among other inflammatory conditions exhibiting sepsis-like symptoms, which is essential for accurate sepsis diagnosis.

Our research aims to bridge this gap by comparing the metabolic profiles of preterm neonates across three groups: neonates without inflammation, neonates with suspected LOS later diagnosed as non-septic, and neonates diagnosed and treated for LOS including both culture-positive and culture-negative cases. In a targeted LC-MS approach, 296 metabolic features covering oxylipins, endocannabinoids, lysophospholipids, free FAs, bile acids, and amines were analyzed in plasma samples to elucidate the similarities and differences in metabolic signatures among these groups. The analyses aim to (i) enhance our understanding of the underlying pathophysiology of sepsis, (ii) identify potential diagnostic biomarkers, and (iii) explore potential sex-specific and pathogen-specific differences in metabolic profiles to provide valuable insights into the heterogeneity of sepsis presentations and responses. These investigations will aid the development of improved diagnostic and tailored therapeutic strategies for LOS in preterm neonates.

2. Methods

2.1 Cohort

The study included 94 preterm neonates (gestational ages: 24–32 weeks) admitted to the Erasmus MC Sophia Children’s Hospital in the Netherlands, between August 2021 and November 2022. A total of 235 samples were categorized into control, suspected sepsis, and follow-up groups. Suspected sepsis samples were obtained upon clinical suspicion of sepsis based on symptoms and heart rate characteristics index,¹⁷ with follow-up samples collected 6–48h later. Control samples, matched for gestational age (± 1 week), sex, and postnatal age (± 4 days), showed no signs of sepsis. The suspected sepsis samples were further classified into “culture-positive sepsis”, “culture-negative sepsis”, or “no sepsis” based on clinical and

laboratory findings. Hereafter, the “no sepsis” group is referred to as “Systemic Inflammation-No Sepsis” (SINS) to underscore the systemic inflammatory response observed in the absence of pathogens that initially prompted sepsis suspicion. An overview of the clinical trajectories and classification criteria for these groups is provided in **Figure 1a** and **Supporting Information S1**.

Analyses were conducted on two datasets: a comprehensive dataset for elucidating sepsis pathophysiology and a single-timepoint (STP) dataset for identifying potential early diagnostic biomarkers. The comprehensive dataset incorporated all available samples, consolidating follow-up samples with their corresponding groups (sepsis or SINS) to enhance statistical power (**Figure 1b**). The STP dataset was curated to include only one sample per patient by excluding follow-up samples, prioritizing first episodes of sepsis cases followed by SINS cases, and including matched controls exclusively from neonates without any occurrences of SINS or sepsis. **Figure S1** illustrates the selection of STP dataset samples from the comprehensive dataset, plotted by the postnatal age at time of sampling.

2.2 Sample Collection

Blood samples (500 μ L) were collected via an arterial line or heel prick, processed immediately to obtain plasma, and partially utilized for serological analyses, including CRP, IL-6, and PCT measurements. The remaining plasma was stored in a biobank at -80°C within 24h, then later retrieved and transported on dry ice to the analytical chemistry laboratory, where it was stored at -80°C until aliquoting for metabolomic analysis (**Supporting Information S1**).

2.3 Metabolomic Data Acquisition

Amino acids, biogenic amines, and signaling lipids were quantified in plasma using ultra-performance liquid chromatography tandem mass spectrometry. Plasma samples were prepared through the addition of internal standards, followed by protein precipitation and derivatization for amines or lipid extraction for signaling lipids. Chromatographic separations were carried out on Agilent and Shimadzu systems equipped with C18 columns, and analytes were detected using multiple reaction monitoring on Sciex QTRAP mass spectrometers. Data acquisition and peak integration were performed using Sciex MultiQuant and Sciex OS software. A detailed description of the experimental protocols is provided in the **Supporting Information S2**.

2.4 Data Preprocessing

Quality control was performed by retaining only metabolites with $<30\%$ relative standard deviation in pooled study samples, $<40\%$ background signal in method blanks, and $<20\%$

missingness. Biologically pertinent metabolite ratios, sums, and means were computed to provide insights into enzyme activities and shifts in metabolic pathways. All data were \log_2 transformed, missing values imputed using the Quantile Regression Imputation of Left-Censored data method,¹⁸ and auto-scaled for multivariable analysis. Further details are provided in **Supporting Information S3**.

2.5 Statistics

All statistical analyses were performed in RStudio (v4.3.1). Linear mixed models (LMMs), ANOVA, and fold change (FC) analyses were applied to the comprehensive dataset to identify metabolic associations with controls, SINS, and sepsis. Two primary LMMs were implemented: (i) the “Inflamed” model, comparing the inflamed groups (SINS + sepsis) to controls, and (ii) the “Sepsis” model, comparing the non-sepsis groups (control + SINS) to sepsis. Additional pairwise comparisons (control vs. SINS (C_SINS model), control vs. sepsis (C_S model), SINS vs. sepsis (SINS_S model)) were used to aid interpretation (**Figure 1c**). LMM results were visualized using volcano plots and compared using forest plots and directed p-value plots, where the directed p-values are the negative logarithm (base 10) of the p-value multiplied with the sign of the estimate. Further analyses investigated the Sepsis model to datasets stratified by sex, pathogen, and blood culture outcome. All models were corrected for confounders identified by Fisher’s exact test for categorical variables, Welch’s t-test for continuous variables, and visual inspection by Principal Component Analysis (PCA).

The STP dataset was investigated using logistic regression, bootstrap-aggregated LASSO logistic regression, spearman and differential correlation analyses. Briefly, logistic regression univariate models were computed for pairwise comparisons (C_SINS, C_S, and SINS_S) to investigate the diagnostic potential of metabolites. Bootstrap-aggregated LASSO logistic regression was used to identify multivariable metabolomic diagnostic models to distinguish between SINS and sepsis at the moment of suspicion. Predictive performance was estimated by averaging metrics across 100 bootstrap iterations. A reduced model based on consistently selected features across bootstraps was evaluated using Leave-One-Out Cross-Validation to derive the Area Under the Receiving Operating Characteristics Curve and compared against inflammatory marker and integrated models using McNemar’s test. Furthermore, spearman and differential correlation analyses were performed to explore the relationship between metabolites and inflammatory markers under SINS and sepsis. A significance threshold of 0.05 was applied to p-values across all statistical analyses. To account for multiple testing in univariate analyses, p-values were adjusted using Benjamini-Hochberg method applying a significance threshold of $q < 0.1$. These corrections accounted for the total number of

metabolic features in univariate tests (n=296). A detailed description of the analyses is provided in **Supporting Information S4**.

2.6 Ethics

The study was approved by the local ethics committee of the Erasmus Medical Centre (MEC-2020-0547). In accordance with standard care protocols, informed parental consent for the utilization of data and residual biomaterial for future medical research was obtained upon patients' admission to the neonatal intensive care unit.

3. Results

3.1 Cohort Characteristics

After quality control, 8 of 235 samples were excluded from analysis; 1 due to diagnostic ambiguity from misclassification, 1 due to insufficient sample volume, and 6 identified as outliers - 4 via the Rosner test based on internal standards and 2 through visual inspection during peak integration and PCA. Of 317 metabolites measured using two assays, 254 met the predefined acceptance criteria, with 208 presenting varying percentages of missingness. Forty metabolites had missing data exceeding 20%, with missingness patterns detailed in **Table S1**. The study included 10 confounders: sample source (artery/capillary), mechanical ventilation, intraventricular hemorrhage, and antibiotic administration within 24h prior to sampling were found to be associated with sepsis outcome, while gestational age, birth weight, postnatal age, sex, oxygen saturation, and proportion of calories provided by total parenteral nutrition were found to influence the metabolite levels.¹⁹⁻²¹ A summary of key demographic and clinical characteristics across both comprehensive and STP datasets, is provided in **Table 1a** and **1b**.

3.2 Differentially regulated metabolites in systemic inflammation and sepsis

The univariate investigation of differential metabolic abundances on the comprehensive dataset revealed significant disruptions in amino acid and lipid metabolism across both the Inflamed and Sepsis models, underscoring the profound impact of systemic inflammation on the neonatal metabolome. There were 91 metabolites statistically significant in the Inflamed model (**Figure 2a**), with 30 metabolites (86.67% signaling lipids) elevated and 61 metabolites (57.38% amines) reduced in the inflamed group (**Table S2**). In the Sepsis model, 96 metabolites showed significant changes (**Figure 2b**), with an increase in 37 metabolites (81.08% signaling lipids) and a decrease in 59 metabolites (59.32% amines) in the sepsis group (**Table S3**). Results from C_SINS, C_S, and SINS_S models are provided in **Figure S2** and **Tables S4-S6**.

Table 1. Demographic and clinical characteristics of the study cohort. The table presents the demographic and clinical characteristics of the (a) comprehensive dataset and (b) single time point dataset, including gestational age, birth weight, current weight, postnatal age, proportion of total parenteral nutrition, oxygen saturation percentage, sex distribution, mechanical ventilation status, sample origin, and incidence of intraventricular hemorrhage. Values are expressed as mean ± standard deviation (sd) for continuous variables and number (percentage) for categorical variables.

Characteristic	Comprehensive Dataset (n=227)					Sepsis (n=85)			
	All (n=227)	Control (n=86)	Systemic Inflammation- No Sepsis (n=56)	Culture- Negative Sepsis (n=42)		Culture-Positive Sepsis (n=43)		Gram-Negative Sepsis (n=14)	
				All (n=85)	Culture- Negative Sepsis (n=42)	All (n=43)	Gram-Positive Sepsis (n=29)	All (n=43)	Gram-Negative Sepsis (n=14)
Gestational Age at Birth in weeks [mean ± sd]	26.67 ± 2.07	26.8 ± 2.01	26.41 ± 1.95	26.71 ± 2.23	26.48 ± 2.29	26.93 ± 2.17	27.17 ± 2.34	26.42 ± 1.74	26.42 ± 1.74
Birthweight in grams [mean ± sd]	891.9 ± 279.45	926.66 ± 259.7	813.04 ± 249.22	908.68 ± 309.06	863.05 ± 277.41	953.26 ± 334.35	978.97 ± 385.16	900 ± 192.69	900 ± 192.69
Current Weight at Sampling in grams [mean ± sd]	1137.89 ± 417.86	1169.76 ± 434.5	1053.54 ± 329.72	1161.24 ± 448.58	1199.05 ± 396.08	1124.3 ± 496.45	1143.45 ± 525.23	1084.64 ± 446.76	1084.64 ± 446.76
Postnatal Age at Sampling in days [mean ± sd]	21.19 ± 18.45	21.03 ± 19.06	21.05 ± 18.78	21.45 ± 17.81	26.76 ± 18.86	16.26 ± 15.21	14.97 ± 13.2	18.93 ± 18.99	18.93 ± 18.99
Proportion of Total Parenteral Nutrition [mean ± sd]	0.38 ± 0.38	0.36 ± 0.36	0.38 ± 0.42	0.4 ± 0.38	0.36 ± 0.42	0.45 ± 0.34	0.48 ± 0.34	0.39 ± 0.35	0.39 ± 0.35
Percentage of Oxygen Level [mean ± sd]	30.13 ± 14.33	26.27 ± 8.28	32.75 ± 9.13	32.31 ± 14.8	31.5 ± 11.47	33.09 ± 17.56	34.55 ± 18.18	30.07 ± 16.42	30.07 ± 16.42
Gender [n (%)]									
Male	91 (40.09)	52 (60.47)	29 (51.79)	55 (64.71)	22 (52.38)	33 (76.74)	22 (75.86)	3 (21.43)	3 (21.43)
Female	136 (59.91)	34 (39.53)	27 (48.21)	30 (35.29)	20 (47.62)	10 (23.26)	7 (24.14)	13 (44.83)	13 (44.83)
Sample Origin [n (%)]									
Artery	15 (22.47)	9 (10.47)	15 (26.79)	27 (31.76)	11 (26.19)	16 (37.21)	16 (57.14)	16 (57.14)	16 (57.14)
Capillary	176 (77.53)	77 (89.53)	41 (73.21)	58 (68.24)	31 (73.81)	27 (62.79)	20 (46.51)	12 (41.38)	12 (41.38)
Mechanical Ventilation [n (%)]	115 (50.66)	58 (67.44)	27 (48.21)	30 (35.29)	10 (23.81)	20 (46.51)	23 (53.49)	17 (58.62)	17 (58.62)
Yes	112 (49.34)	28 (32.56)	29 (51.79)	55 (64.71)	32 (76.19)	23 (53.49)	23 (53.49)	17 (58.62)	17 (58.62)
No	166 (73.13)	71 (82.56)	46 (82.14)	49 (57.65)	28 (66.67)	21 (48.84)	13 (44.83)	8 (57.14)	8 (57.14)
Intraventricular Hemorrhage [n (%)]	61 (26.87)	15 (17.44)	10 (17.86)	36 (42.35)	14 (33.33)	22 (51.16)	16 (55.17)	6 (42.86)	6 (42.86)
Yes									
No									

Characteristic	Single Time Point Dataset (n=92)				Sepsis (n=40)					
	All (n=92)	Control (n=35)	Systemic Inflammation- No Sepsis (n=17)	Culture- Negative Sepsis (n=21)	All (n=40)		Culture-Positive Sepsis (n=19)		Gram-Negative Sepsis (n=7)	
					All (n=40)	Culture- Negative Sepsis (n=21)	All (n=19)	Gram-Positive Sepsis (n=12)	All (n=7)	Gram-Negative Sepsis (n=7)
Gestational Age at Birth in weeks [mean ± sd]	27.09 ± 2.1	27.67 ± 2.09	27.23 ± 1.7	26.51 ± 2.17	26.44 ± 2.09	26.61 ± 2.3	27.02 ± 2.56	25.9 ± 1.71	25.9 ± 1.71	
Birthweight in grams [mean ± sd]	958.85 ± 289.58	1055.74 ± 269.66	908.82 ± 235.95	895.32 ± 309.49	844.9 ± 260.82	951.05 ± 354.54	1022.92 ± 414.71	827.86 ± 183.69	827.86 ± 183.69	
Current Weight at Sampling in grams [mean ± sd]	1118.16 ± 432.58	1228.29 ± 488.98	968.88 ± 272.66	1085.25 ± 419.5	1080 ± 301.51	1091.05 ± 529.35	1085 ± 502.77	1101.43 ± 614.01	1101.43 ± 614.01	
Postnatal Age at Sampling in days [mean ± sd]	16.49 ± 16.92	16.6 ± 19.85	11.35 ± 9.33	18.58 ± 16.53	22.38 ± 14.85	14.37 ± 17.64	10.58 ± 8.9	20.86 ± 26.66	20.86 ± 26.66	
Proportion of Total Parenteral Nutrition [mean ± sd]	0.39 ± 0.35	0.44 ± 0.35	0.43 ± 0.39	0.32 ± 0.34	0.26 ± 0.37	0.39 ± 0.32	0.44 ± 0.33	0.3 ± 0.3	0.3 ± 0.3	
Percentage of Oxygen Level [mean ± sd]	28.27 ± 12.33	24.23 ± 7.99	28 ± 15.96	31.92 ± 12.89	30.86 ± 9.89	33.11 ± 15.76	32.17 ± 12.45	34.71 ± 21.36	34.71 ± 21.36	
Gender [n (%)]										
Male	52 (56.52)	18 (51.43)	8 (47.06)	26 (65)	12 (57.14)	14 (73.68)	9 (75)	5 (71.43)	5 (71.43)	
Female	40 (43.48)	17 (48.57)	9 (52.94)	16 (45)	9 (42.86)	5 (26.32)	6 (50)	2 (28.57)	2 (28.57)	
Sample Origin [n (%)]										
Artery	19 (20.65)	3 (8.57)	4 (23.53)	12 (30)	5 (23.81)	7 (36.84)	6 (50)	1 (14.29)	1 (14.29)	
Capillary	73 (79.35)	32 (91.43)	13 (76.47)	28 (70)	16 (76.19)	12 (63.16)	6 (50)	6 (85.71)	6 (85.71)	
Mechanical Ventilation [n (%)]	54 (58.7)	26 (74.29)	11 (64.71)	17 (42.5)	13 (61.9)	9 (47.37)	5 (41.67)	4 (57.14)	4 (57.14)	
Yes	38 (41.3)	9 (25.71)	6 (35.29)	22 (57.5)	13 (61.9)	10 (52.63)	7 (58.33)	3 (42.86)	3 (42.86)	
No	68 (73.91)	31 (88.57)	14 (82.35)	22 (57.5)	13 (61.9)	10 (52.63)	5 (41.67)	5 (71.43)	5 (71.43)	
Intraventricular Hemorrhage [n (%)]	24 (26.09)	4 (11.43)	3 (17.65)	17 (42.5)	8 (38.1)	9 (47.37)	7 (58.33)	2 (28.57)	2 (28.57)	
Yes										
No										

Figure 3 illustrates a comprehensive comparison of key metabolite changes across all five models. ANOVA and fold change (FC) analyses further revealed distinct metabolic patterns across control, SINS, and sepsis groups.

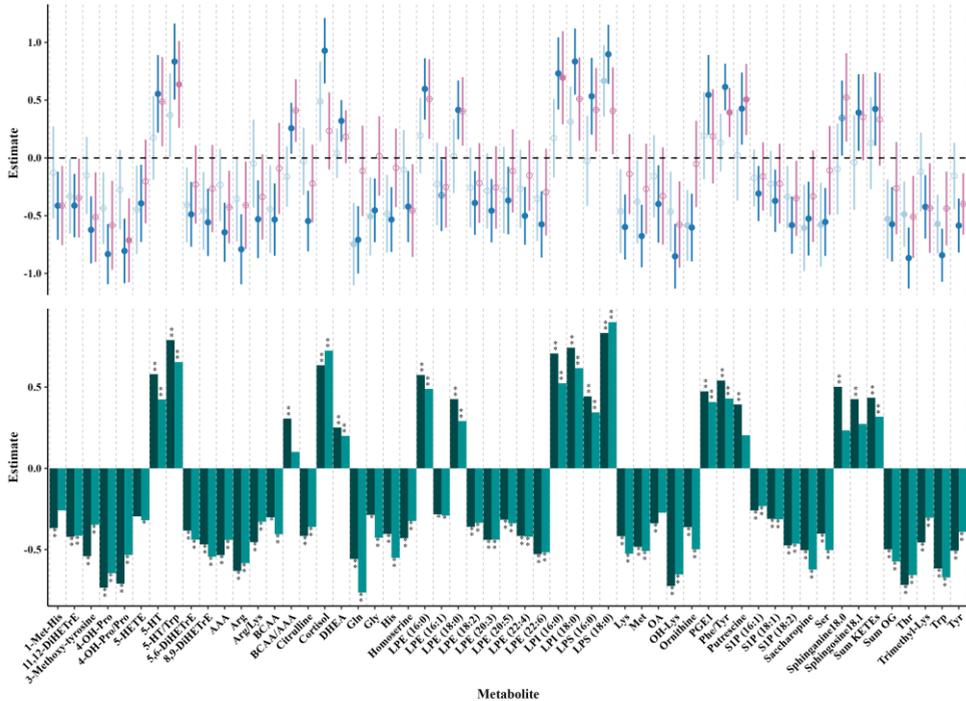


Figure 3. Comparative assessment of metabolic changes in inflammatory and septic conditions. The figure presents a comprehensive analysis of metabolite estimates derived from different linear mixed-effect models. The bottom panel shows bar plots comparing the estimates from the Inflamed (green) and Sepsis (dark green) model for each metabolite. The top panel features a forest plot displaying the estimates and confidence intervals of the additional models: C_S_SINS (light blue), C_S (blue) and SINS_S (pink). The dual-panel visualization allows for a comprehensive comparison of how metabolites are differentially regulated across these models, highlighting the similarities and differences in metabolite behavior in response to systemic inflammation-no sepsis and sepsis. Metabolite significance before and after FDR correction is depicted with different shapes: significant after correction (filled circle or **), significant before correction (circle with a plus or *), and not significant (circle or nothing). C_S_SINS = control versus systemic inflammation-no sepsis; C_S = control versus sepsis; SINS_S = systemic inflammation-no sepsis versus sepsis; FDR = False Discovery Rate.

3.2.1. Etiology-independent metabolic signatures of systemic inflammation

Among the 79 metabolites common between the Inflamed and Sepsis models, 30 demonstrated highly comparable levels with similar FC in both SINS and sepsis groups compared to the control (**Figure 4a**, **Table S7**). Notably, amino acids, including glycine, glutamine, lysine, histidine, serine, saccharopine, ornithine, and BCAA were consistently downregulated in both C_S_SINS and C_S models, with FC ranging from 0.72-0.91 for SINS and 0.74-0.90 for sepsis, indicating uniform trends across both inflammatory conditions. Similarly, arachidonic acid derivatives (5,6-DiHETrE, 8,9-DiHETrE, 11,12-DiHETrE, 5-

Chapter III

HETE; FC: 0.55-0.77), monounsaturated sphingosine-1-phosphates (S1P(16:1), S1P(18:1); FC: 0.73-0.80), and unsaturated LPEs (LPE(16:1), LPE(18:2), LPE(20:3), LPE(20:5), LPE(22:4), LPE(22:6); FC: 0.68-0.89) exhibited decreased levels in both inflammatory groups. However, the regulation of S1Ps and LPEs in C_SINS model did not reach the conventional threshold of $p < 0.05$, likely due to the smaller sample size and greater variability within the SINS group.

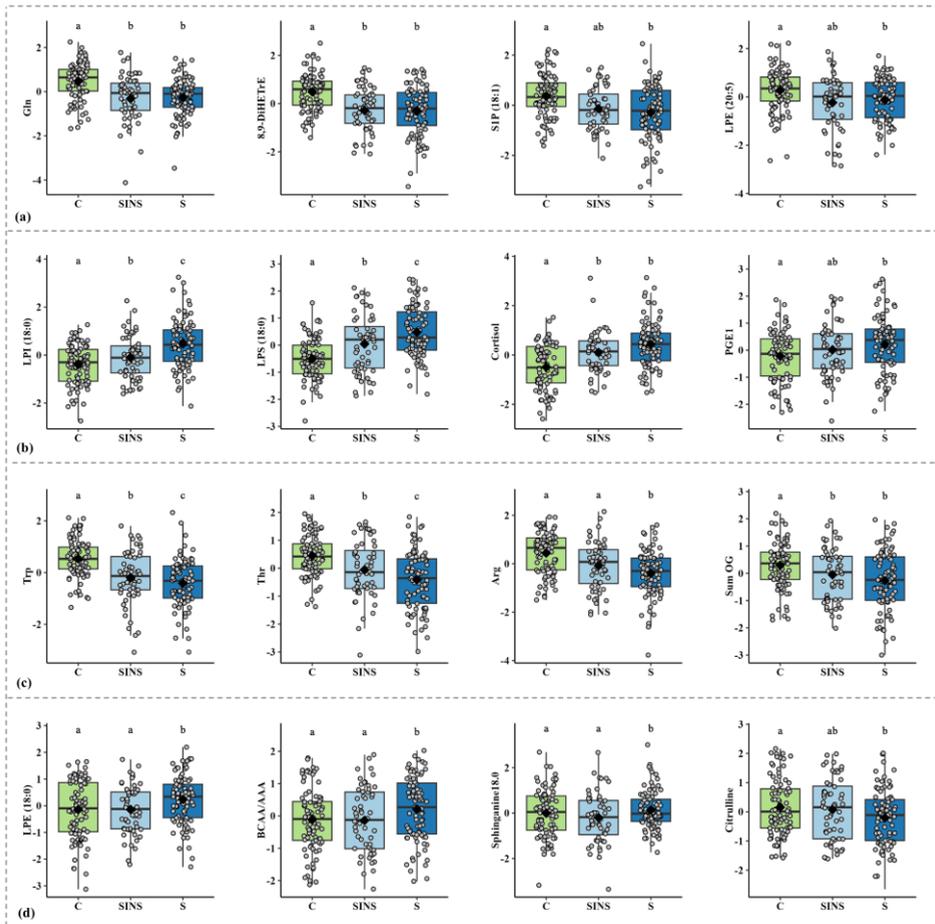


Figure 4. Metabolite level trends across control, systemic inflammation-no sepsis, and sepsis groups. The figure presents a series of boxplots illustrating the distribution of metabolite levels prior to confounder correction, highlighting specific trends across the three groups: (a) Metabolites with similar levels in both SINS and sepsis compared to control, (b) Metabolites exhibiting an increasing trend from control to SINS to sepsis, (c) Metabolites showing a decreasing trend from control to SINS to sepsis, and (d) Metabolites specifically upregulated or downregulated only in sepsis, with similar levels in control and SINS. In each boxplot, the central line represents the median, with box edges denoting the interquartile range. Individual data points represent samples, and the black diamond represents the mean. The letters denote significance between groups from the linear-mixed effect models: shared letters indicate no significant difference, while unique letters indicate significant difference. C = Control (green); SINS = Systemic Inflammation-No Sepsis (light blue); S = Sepsis (blue).

3.2.2 Metabolic markers of enhanced immune dysregulation in sepsis

Several metabolites demonstrated a progressive increase (**Figure 4b**) or decrease (**Figure 4c**) in their levels from control to SINS to sepsis (**Table S7**). Notably, LPS(18:0) and LPI(18:1) showed a consistent upward trend with increasing severity of inflammation, while tryptophan, threonine, hydroxylysine, 4-hydroxyproline and S1P(18:2) exhibited a consistent downward trend, with $p < 0.05$ in both C_SINS and SINS_S models. Additionally, cortisol (C_SINS FC: 2.4; SINS_S FC: 1.5), arginine (C_SINS FC: 0.79; SINS_S FC: 0.84) and sum of OG (C_SINS FC: 0.85; SINS_S FC: 0.92) displayed larger fold changes from control to SINS than SINS to sepsis. Alternatively, fold changes in tyrosine (C_SINS FC: 0.87; SINS_S FC: 0.79), 3-methoxy-tyrosine (C_SINS FC: 0.91; SINS_S FC: 0.82), AAA (C_SINS FC: 0.91; SINS_S FC: 0.85), and 4-hydroxyproline/proline (C_SINS FC: 0.88; SINS_S FC: 0.84) were higher in SINS to sepsis. Furthermore, PGE1 and arginine/lysine showed an increasing and decreasing trend, respectively, but achieved significance of $p < 0.05$ only in the extreme comparison of control to sepsis, as opposed to their subtle gradual shifts from control to SINS or SINS to sepsis.

3.2.3 Sepsis-specific and SINS-specific metabolic dysregulations

In the analysis of the Inflamed model, several metabolites showed statistical significance driven exclusively by the sepsis group, with similar levels in control and SINS but distinct differential regulation in sepsis, suggesting their potential as sepsis-specific biomarkers (**Table S7, Figure 4d**). Notably, serotonin (FC: 2.27), saturated lysophospholipids (LPE(16:0), LPE(18:0), LPI(16:0), LPS(16:0); FC: 1.04-1.35), DHEA (FC: 1.12), and sum of KETEs (FC: 1.32) were elevated, while citrulline (FC: 0.83), homoserine (FC: 0.89), and trimethyl lysine (FC: 0.95), were decreased in sepsis. Additional sepsis-specific signatures identified from the Sepsis model included increased levels of putrescine (FC: 1.69), sphinganine(18:0) (FC: 1.04), sphingosine(18:1) (FC: 1.00), and BCAA/AAA (FC: 1.13), alongside reductions in oleic acid (FC: 0.95) and 1-methyl-histidine (FC: 0.96). However, the association of LPS(16:0), trimethyl-lysine, sphinganine(18:0), sphingosine(18:1), oleic acid and 1-methyl-histidine with sepsis became significant only after correction for confounders.

PGF1alpha was observed to be significantly downregulated exclusively in the SINS group when compared to the controls, underscoring its potential as a SINS-specific biomarker (**Figure S3a**). Additionally, when stratifying the sepsis group by blood culture outcome, PGF1alpha was significantly downregulated in culture-negative sepsis, whereas culture-positive sepsis exhibited an upward trend (**Figure S3b, Table S8**).

3.3 Sex-specific phenotypic distinction in inflammatory response to sepsis

Sex stratification on the comprehensive dataset resulted in a male cohort (n=54, 136 samples) with 55 sepsis samples (40.44%), and a female cohort (n=30, 91 samples) with 30 sepsis samples (32.97%). The sex-stratified Sepsis models identified a pro-inflammatory phenotype in males, characterized by elevated prostaglandins (PGE1 (Estimate=0.46), PGE2 (Estimate=0.47), PGF2alpha (Estimate=0.61), delta-17,6-keto-PGF1alpha (Estimate=0.52)), and decreased DiHETrEs (Estimate= -0.49- -0.69) and sum of OG (Estimate= -0.70). Additionally, increased levels of serotonin (Estimate=0.82), GABA (Estimate=0.45), sphinganine(18:0) (Estimate=0.55), and sphingosine(18:1) (Estimate=0.45), as well as decreased levels of trimethyl lysine (Estimate= -0.55), and homoserine (Estimate= -0.46) were found to be exclusively and significantly associated with sepsis in males. These associations were identified only after confounder correction; therefore, raw FC are not reported. Females, on the other hand, exhibited an anti-inflammatory phenotype, characterized by increased omega-3 FAs and their metabolites, including EPA (Estimate=0.35) and its derivatives (9-HEPE (Estimate=0.42), 12-HEPE (Estimate=0.52), 15-HEPE (Estimate=0.52), 18-HEPE (Estimate=0.54)), and DHA metabolites (16-HDoHE (Estimate=0.38), 17-HDoHE (Estimate=0.42), 20-HDoHE (Estimate=0.47)). Increased levels of DHEA (Estimate=0.43), sum of KETEs (Estimate=0.64), and AEA (Estimate=0.41), as well as decreased levels of citrulline (Estimate= -0.65) and histidine (Estimate= -0.71), were also found to be predominantly driven by females. Although some female-driven metabolites did not attain statistical significance of $q < 0.1$, likely due to the smaller cohort size, consistent trends within metabolite classes ($p < 0.05$) support these observed sex-specific differences. **Figure 5a** illustrates the sex-specific response to sepsis in the two genders with a more detailed comparison of metabolites including significance values and shared metabolites across sexes presented in **Figure S4a** and **Table S9**.

3.4 Pathogen-driven metabolomic heterogeneity in sepsis

Of the 43 culture-positive sepsis samples in the comprehensive dataset, 29 were associated with gram-positive bacteria and 14 with gram-negative bacteria, with similar male-to-female ratio, indicating no sex bias in the stratification analysis (Fisher's exact test $p = 1$). Pathogen-stratification in the Sepsis models elucidated metabolic dysregulations uniquely associated with each pathogen type (**Figure 5b**). An extensive comparison of metabolite profiles, including p-values and shared metabolites across both bacterial groups, is provided in **Figure S4b** and **Table S10**. Patients with gram-negative sepsis exhibited significantly increased levels of COX enzyme induced metabolites (PGE1 (Estimate=1.03), PGE2 (Estimate=0.94), PGF2alpha (Estimate=0.87)) and reduced levels of endocannabinoids (sum of OG (Estimate= -0.93), sum of LG (Estimate= -0.64)) and citrulline (Estimate= -0.80). Further, serotonin (Estimate=0.62), putrescine (Estimate=0.61), sum of KETEs (Estimate=0.63), 4-

hydroxyproline/proline (Estimate= -0.64), and arginine/lysine (Estimate= -0.62) were found to be predominantly driven by gram-negative sepsis with $p < 0.05$ ($q > 0.1$). On the contrary, gram-positive sepsis was characterized by decreased levels of CYP enzyme induced DiHETrEs (Estimate= -0.65- -0.89), unsaturated lysophospholipids, including LPEs (Estimate= -0.45- -0.81) and LPAs (Estimate= -0.41- -0.65), and increased levels of cortisol (Estimate= 0.56), DHEA (Estimate= 0.26), and omega-3/omega-6 FA ratio (Estimate= 0.31). Some LPEs and LPAs, DHEA, and omega-3/omega-6 FA ratio did not achieve the statistical significance of $q < 0.1$.

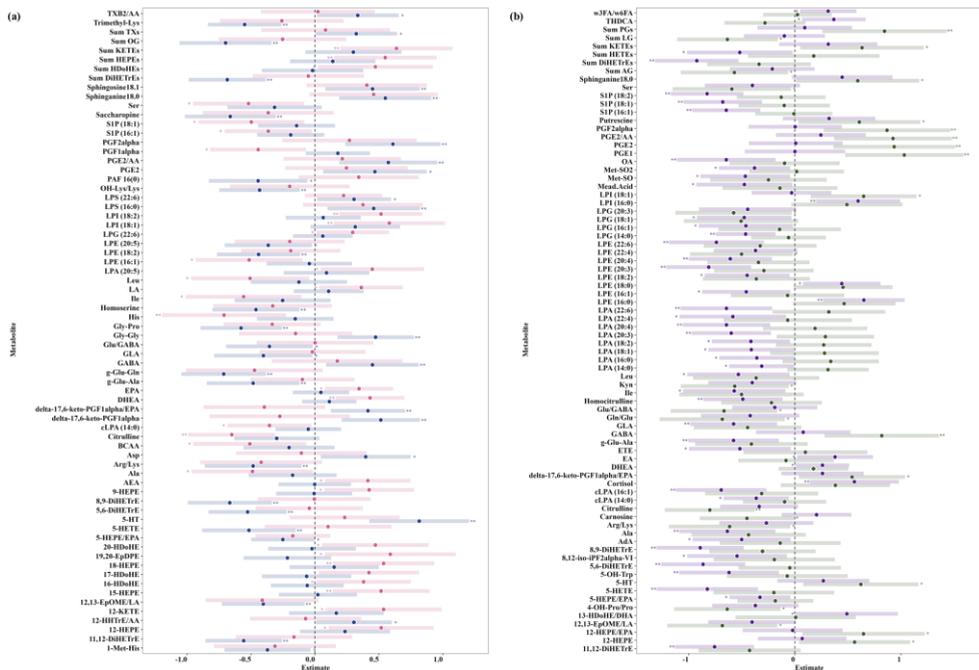


Figure 5. Forest plots of metabolite estimates in sex and pathogen-stratified sepsis models. The figure presents forest plots illustrating the estimates with significance, before and after FDR correction, of metabolite levels in linear-mixed effect sepsis models stratified by sex and pathogen type. Confidence intervals are represented by the horizontal bars. The left panel (a) shows the estimates for male (*dark blue*) and female (*pink*) sepsis models, while the right panel (b) displays the estimates for gram-positive (*purple*) and gram-negative (*dark green*) sepsis models. These plots highlight the differences in metabolite regulation influenced by sex and pathogen type, providing a comprehensive comparison of the metabolic responses across these stratified groups. FDR = False Discovery Rate; Significance after correction = “***”; Significance before correction = “**”; Not significant = “”

3.5 Diagnostic potential of metabolites for early and accurate detection of sepsis

The logistic regression models identified 26 significant metabolites ($q < 0.1$) in the C_S model, while no significant hits were observed in the C_SINS and SINS_S models, likely due to the limited sample size in the STP dataset. A comparison of metabolites with $p < 0.05$

between the C_S and C_SINS models revealed that 31 of the 61 metabolites were exclusively associated with sepsis (**Figure S5a**), with a substantial overlap observed with LMM results. Additionally, analysis of the SINS_S model identified metabolites such as cortisol, putrescine, 11beta-PGF2alpha/AA, S1P(18 :2), and LPA(20.4) as potential biomarkers for distinguishing SINS from sepsis (**Figure S5b**). Details of these results are documented in **Supporting Information S5** and **Tables S11-S13**.

The predictive performance of the metabolomic diagnostic framework for distinguishing SINS from sepsis at the point of clinical suspicion, as estimated using bootstrap-aggregated LASSO logistic regression across 100 iterations, yielded a mean AUC of 0.61, sensitivity of 0.69 and specificity of 0.66. Detailed performance metrics for each iteration are provided in Supplementary **Table S14**. Feature selection stability analysis identified five metabolites, including 11-beta-PGF2alpha, o-acetyl-serine, PGE1, 8-iso-PGF3alpha, and taurine, which were consistently selected in over 45% of the bootstrap models. The multivariable logistic regression model constructed using these 5 metabolites demonstrated a good discriminatory performance, with an AUC of 0.75, sensitivity of 0.82, specificity of 0.73, PPV of 0.9, and F1 score of 0.86. In contrast, models based on individual inflammatory markers showed limited diagnostic utility (AUCs: CRP=0.53, IL-6=0.59, PCT=0.55), and their combination further reduced performance (AUC:0.49). However, integration of the metabolite panel to the individual inflammatory markers led to improved classification. The highest diagnostic performance was achieved by combining the metabolite panel with IL6 (McNemar p-value: 0.01), resulting in an AUC of 0.79, sensitivity of 0.85, specificity of 0.82, PPV of 0.93, and F1 score of 0.89. Combinations with either CRP (McNemar p-value: 0.02) or PCT (McNemar p-value: 0.002) yielded an AUC of 0.74. Receiver operating characteristic curve and model parameters are provided in **Figure 6** and **Table S15**.

Spearman correlation analyses revealed differential correlations between diagnostic panel metabolites and inflammatory markers in SINS and sepsis, as illustrated in **Figure S6**. Notably, o-acetyl-serine displayed a strong positive correlation with CRP ($\rho_s = 0.66$, $p = 0.03$) and PCT ($\rho_s = 0.71$, $p = 0.01$) in SINS, whereas no correlation was observed in sepsis (CRP: $\rho_s = -0.01$, $p = 0.94$; PCT: $\rho_s = -0.24$, $p = 0.19$). Similarly, 8-iso-PGF3alpha ($\rho_s = -0.76$, $p = 0.0092$) exhibited a negative correlation with IL6 in SINS, but no correlation in sepsis ($\rho_s = -0.1$, $p = 0.58$).

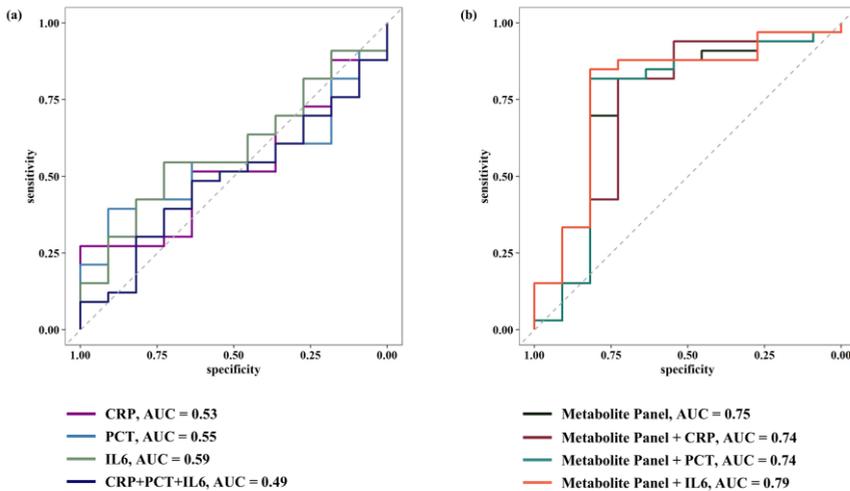


Figure 6. Area under the receiver operating characteristic curves for diagnostic models differentiating systemic inflammation-no sepsis from sepsis at moment of suspicion. The figure presents the receiver operating characteristic curves with the area under the curve for (a) individual and combined routine inflammatory marker models and (b) metabolomic and integrated models. The metabolite panel includes 5 metabolites: 11beta-PGF2alpha, o-acetyl serine, PGE1, 8-iso-PGF3alpha, and taurine. The area under the curve values obtained from the leave-one-out cross-validation demonstrates the diagnostic performance of these models in distinguishing between systemic inflammation-no sepsis and sepsis at the moment of suspicion.

4. Discussion

To the best of our knowledge, this is the first metabolomic study conducted on preterm neonates that delineates the similarities and differences between SINS and sepsis using well-defined patient subgroups for analysis. The study further explores the potential of metabolomics to unravel the observed clinical disparities in sex-specific and pathogen-specific sepsis presentations, facilitating potential personalized treatment strategies. A comprehensive overview of the key findings in the study summarizing the results across all models, is shown in **Figure 7**.

The uniform downregulation of several amino acids and signaling lipids in SINS and sepsis reflects the body's fundamental response mechanism to systemic inflammation, regardless of the causative trigger. These findings underscore the tremendous metabolic stress experienced by the infants, driven by increased metabolic demands and disruptions in synthesis or recycling pathways. Reduced amino acid levels suggest impairments in protein synthesis and metabolism, essential for maintaining immune function and cellular repair.^{22,23} The significant decrease in glutamine may be attributed to its heightened utilization by proliferating immune cells, a hallmark of systemic inflammation.²² Similarly, reduced BCAAs, key activators of the mTORC1 pathway for protein synthesis, indicate a shift

towards protein catabolism, often linked to muscle wasting in inflammatory conditions.^{23,24} Further, reduced levels of unsaturated LPEs and histidine indicate oxidative stress and redox imbalance, potentially driven by reactive oxygen species oxidizing the LPE double bonds and depleting antioxidant reserves.²⁵ The downregulation of metabolites with anti-inflammatory properties, such as glycine,²⁶ serine,²⁷ and DiHETrEs,²⁸ reflects an inadequate compensatory response to heightened pro-inflammation. The depletion of lysine and glycine, both essential for collagen production, indicates impaired tissue repair capacity.^{29,30} These uniform metabolic perturbations underscore the challenge in differentiating systemic inflammation arising from infectious vs. non-infectious causes and offer promising targets for restoring metabolic balance and improving patient outcomes in systemic inflammation.

Metabolites exhibiting progressive trends from control to SINS to sepsis deepen the understanding of pathways associated with escalating inflammatory burden. The increasing severity of inflammation necessitates higher production of acute phase proteins, imposing a considerable metabolic strain reflected in, amongst others, the declining levels of threonine, which is essential for acute-phase response and gut barrier integrity.³¹ The dysregulation of S1Ps, particularly declining S1P(18:2) levels which are lowest in sepsis, further compromises intestinal and endothelial integrity, promoting vascular permeability, leakage, and edema that contribute to sepsis-induced organ failure.³² Inhibition of S1P degradation has shown tissue-protective effects in sepsis, reducing severity and improving survival by enhancing disease tolerance.³³ The declining arginine levels, attributed to increased nitric oxide production and reduced *de novo* synthesis as widely reported in sepsis studies, may impair vascular function, neurotransmission, and host defenses.³⁴⁻³⁷ Arginine insufficiency has been hypothesized as a key factor impairing immune responses in preterm neonates during infections.³⁸ High cortisol levels promote pro-inflammatory cytokine production thus exacerbating inflammation in sepsis.³⁹ While arginine and cortisol changes primarily reflect inflammatory responses, metabolites such as tyrosine and 4-hydroxyproline/proline demonstrate more pronounced changes in response to infection. Decreased tyrosine levels in sepsis may result from increased utilization for catecholamine synthesis or impaired conversion from phenylalanine due to enzymatic dysfunction.^{40,41} Further, the lower 4-hydroxyproline/proline ratio reflects higher tissue damage in sepsis, as 4-hydroxyproline is essential for collagen stability.⁴² Overall, these trends highlight the greater severity and deterioration in sepsis compared to SINS, offering insights into potential diagnostic thresholds and therapeutic targets.

Exclusively altered metabolites in the sepsis group provide crucial insights into sepsis pathophysiology and potential diagnostic biomarkers. For instance, elevated serotonin levels have been linked to several sepsis associated complications ranging from enhancing bacterial virulence to fostering a pro-thrombotic environment leading to ischemia and organ

failure.⁴³⁻⁴⁵ Exacerbated depletion of platelets and coagulation factors has been identified as an independent risk factor for neonatal sepsis-associated mortality.⁴⁶ Elevated saturated lysoglycerophospholipids in sepsis reflect heightened phospholipase A2 enzyme activity, which hydrolyzes membrane phospholipids to produce lysoglycerophospholipids and free FAs.⁴⁷ These saturated lipid species accumulate under oxidative stress, likely due to their enhanced stability and resistance to peroxidation from their lack of double bonds. Elevated putrescine, driven by enhanced ornithine decarboxylase enzyme activity, indicates the body's attempt to regulate immune function and cellular repair in sepsis.^{48,49} This shift in ornithine metabolism reduces citrulline levels, reflecting the impaired *de novo* arginine and nitric oxide production.³⁶ Similarly, higher sphinganine(18:0) in sepsis represents a protective mechanism against intestinal barrier injury.⁵⁰ Furthermore, the significant downregulation of PGF1alpha in SINS, mirrored in culture-negative sepsis group and contrasted by an opposite trend in culture-positive sepsis, suggests that the presence of detectable pathogens may distinctly influence PGF1alpha regulation. The absence of detectable pathogens in culture-negative sepsis cases raises the possibility of misclassified SINS, potentially driving the observed downregulation in the culture-negative sepsis group. Therefore, PGF1alpha could be a potential marker to distinguish between SINS and true sepsis cases in the absence of detectable pathogens. Collectively, these metabolic changes illustrate the unique and complex adaptive responses in sepsis, highlighting the differences between SINS and sepsis.

Sex-stratified analysis identified metabolites significantly associated with sepsis in either male or female preterm neonates, suggesting potential sex-specific immune responses. In males, the decreased levels of anti-inflammatory DiHETrEs and OGs, coupled with elevated pro-inflammatory prostaglandins such as PGE2 and PGF2alpha, suggest a skewed inflammatory balance toward a heightened pro-inflammatory state. These arachidonic acid-derived eicosanoids are well-established mediators of inflammation and have been linked to severe inflammatory responses.⁵¹ Elevated serotonin levels observed in males may further exacerbate this pro-inflammatory milieu by promoting platelet activation and thrombus formation, which is consistent with clinical data showing a greater predisposition of males to severe sepsis outcomes and complications, including disseminated intravascular coagulation. Meanwhile, females exhibited increased levels of w3FAs EPA and DHA, their metabolites (HEPEs, HDoHEs), and ethanolamine endocannabinoids, which are known to resolve inflammation, modulate immune cell activity, and maintain homeostasis.⁵² The enhanced production of these metabolites, potentially driven by hormonal or genetic factors, may reflect a protective mechanism that mitigates the severity of sepsis, explaining the more robust and controlled inflammatory response and better outcomes observed in female neonates.⁵³⁻⁵⁵ While these observations align with reported sexual dimorphism in infectious

diseases, interaction testing between sexes were not performed due to limited sample size.⁵⁶ Nonetheless, our sex-stratified models highlight biologically plausible, sex-specific metabolic associations that may contribute to differences in sepsis susceptibility and outcomes, and offer a foundation for future studies exploring sex-informed diagnostic or therapeutic strategies.

Pathogen-stratified analyses identified metabolites significantly associated with sepsis in either gram-positive or gram-negative bacterial infections, suggesting distinct metabolic responses to different causative pathogens. In gram-negative sepsis, elevated levels of COX enzyme-induced metabolites such as PGE2 and PGF2alpha were observed, consistent with a previous study reporting stronger PGE2 production in human monocytes in response to gram-negative bacteria than gram-positive bacteria.⁵⁷ The concurrent reduction in glycerol endocannabinoids suggest a disrupted endocannabinoid system which is crucial for immune regulation.⁵⁸ Elevated levels of serotonin, putrescine, and sum of KETEs further reflect severe clinical outcomes and tissue damage. Meanwhile, gram-positive sepsis was characterized by decreased CYP enzyme-induced metabolites like DiHETrEs and unsaturated LPEs and LPAs, suggesting disrupted FA metabolism and signaling.⁵⁹ Interestingly, increased levels of DHEA and w3FA/w6FA ratio were observed, potentially reflecting adaptive immune regulatory responses in gram-positive sepsis. These differences between gram-positive and gram-negative bacterial sepsis may arise from the rapid clinical presentation of the latter, while the subtler symptoms of the former often delay diagnosis. Alternatively, these differences may reflect distinct immune signaling mechanisms, as lipopolysaccharides from gram-negative bacterial outer membrane activate toll-like receptor 4 (TLR4), triggering potent immune responses, while the peptidoglycan cell wall of gram-positive bacteria predominantly interact with TLR2/TLR6 heterodimer.⁶⁰ These findings suggest pathogen-specific metabolic profiles, which may serve as potential biomarkers for early identification of pathogens or tailored therapeutic targets for effective and personalized interventions, reducing unnecessary broad-spectrum antibiotic use.

The multivariable model comprising 11-beta-PGF2alpha, o-acetyl-serine, PGE1, 8-iso-PGF3alpha, and taurine demonstrated good sensitivity and specificity in distinguishing SINS from sepsis at the moment of suspicion. In contrast, inflammatory marker models showed limited diagnostic utility, underscoring the inadequacy of relying solely on routine clinical biomarkers, which aligns with clinical observations where blood cultures and follow-up samples are required for accurate diagnosis. The integration of inflammatory markers with the metabolic panel significantly improved diagnostic performance, emphasizing the synergistic value of combining diverse biomarker types. The model integrating the metabolic

panel with IL-6 and achieving an AUC of 0.79, with a sensitivity of 0.85 and a specificity of 0.82, reflect both robust detection of true sepsis cases and effective reduction of false positives. This balanced diagnostic profile enhances clinical utility by supporting timely recognition of sepsis while minimizing unnecessary treatment. When used in conjunction with clinical assessment, such an integrated biomarker approach holds promise for improving diagnostic precision in neonatal sepsis and guiding more targeted therapeutic interventions.

The results presented in the study align with known biological mechanisms and clinical observations, but caution is advised, as validation in a larger, more balanced cohort is necessary. However, obtaining an appropriately sized validation cohort may be challenging as preterm neonates are a particularly vulnerable population. Despite the comprehensive dataset having a good sample size, the power is reduced in the STP dataset and the unbalanced datasets created for the stratified analyses. The stratification analyses were thus performed to elucidate metabolic changes rather than identify diagnostic biomarkers for sex- or pathogen-specific treatments. However, the strong differences between the groups suggest potential diagnostic utility and avenues for targeted treatments upon further validation. Additionally, it is crucial to investigate whether sex-specific or universal biomarkers offer the best approach for diagnosing sepsis in both sexes. The ambiguity surrounding culture-negative sepsis introduces heterogeneity to the sepsis group. This complexity underscores the importance of validation to delineate true sepsis-related metabolic alterations from other inflammatory conditions. Future work should focus on validation of the multivariable model to accurately assess diagnostic accuracy, reproducibility, and clinical utility in larger cohorts over multiple centers. Additionally, these findings need to be translated into routine clinical practice which requires robust, portable, user-friendly, and cost-effective devices capable of rapid and accurate metabolite quantification. With continued collaboration between academia, technology developers, clinicians, and regulatory bodies, the findings of this study hold significant potential in paving the way for bedside metabolomics-based diagnostics.

5. Conclusion

In conclusion, this study provides a pivotal advancement in the understanding of late-onset sepsis in preterm neonates, with the potential to fundamentally alter the current diagnostic and treatment landscape. The application of metabolomics to distinguish between SINS and sepsis at the moment of suspicion is a critical breakthrough. Accurate identification of SINS could enable clinicians to align treatment decisions with the actual inflammatory status of the neonate, reserving antibiotics for confirmed infections and mitigating risks such as antibiotic resistance, adverse drug reactions, and microbiome disruption. The sex- and pathogen-

specific insights from this study further highlight the potential for targeted therapies, including the use of narrow-spectrum antibiotics to enhance treatment precision and efficacy, marking a substantial improvement over the current reliance on empirical broad-spectrum antibiotic use. Personalized interventions based on the neonate's metabolic profile could improve outcomes while reducing the limitations of a one-size-fits-all strategy. Additionally, these findings could help clinicians predict which infants are at a greater risk of severe outcomes, allowing for closer monitoring and earlier intervention in high-risk cases. Clinically, integrating metabolomics into routine diagnostics could result in the development of rapid, bedside tests that provide actionable insights within hours. Ultimately, this metabolomics-driven approach could reshape the future of neonatal sepsis management, offering a new standard of care that enhances survival, reduces antibiotic misuse, and provides preterm neonates with a better chance at a healthy start in life.

6. Declarations

6.1 Author Contributions

Guarantors: IKMR, TH; Study conception: HRT, IKMR, TH; Data acquisition and curation: HRT, SH, MUT, JJBG, CNvK; Data analysis: MUT; Visualization: MUT; Manuscript drafting: MUT, AK; Critical revision of manuscript: MUT, AK, HRT, IKMR, BW, TH. All authors had access to data and MUT, AK, and HRT verified the data. The corresponding author attests that all listed authors meet authorship criteria and that no others meeting the criteria have been omitted.

6.2 Conflicts of Interest

The authors have declared no conflict of interest.

6.3 Acknowledgements

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Exposome-Scan which is part of 'Building the Infrastructure for Exposome Research: Exposome-Scan' project (NWO, Project 175.2019.032) under the program 'Investment Grant NWO Large'. Furthermore, we acknowledge funding of the European Funds for the Regional Development (Kansen voor West II: Phenomix Fieldlab).

6.5 Data Sharing Statement

All processed metabolomics data (peak area ratios derived from SCIEX software) and curated metadata are available in a publicly accessible GitHub repository: Manchu1205/MOMETA-Study. The repository also contains the complete analysis pipeline, including preprocessing scripts, statistical modeling code, and figure generation workflows, to ensure full transparency and reproducibility of the findings. In addition, raw LC-MS files and associated metadata have also been deposited to the MetaboLights repository under the study accession number MTBLS10665 (www.ebi.ac.uk/metabolights/MTBLS10665).

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Chapter III

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Supplementary Material

Supplementary Information

S1. Cohort Group Definitions and Sample Processing

- Culture-positive sepsis: samples with confirmed gram-positive or gram-negative bacteria in blood cultures.
- Culture-negative sepsis: samples where blood cultures were negative, yet sepsis symptoms persisted. These are defined by (a) CRP levels exceeding 10 mg/L within 2 days after blood culture, (b) administration of antibiotic therapy longer than 5 days (or intention to treat longer), and (c) clinical symptoms of sepsis assessed by the treating physician.
- No sepsis or SINS: samples from neonates initially displaying symptoms of sepsis with subsequent reassuring clinical status (no/mild symptoms) and negative blood cultures.

The sample collection process entailed acquiring 500 μL of lithium-heparin blood from neonates either through an arterial line or the heel prick technique. The blood sample was centrifuged at 3,000g for 5 min at room temperature to obtain plasma. A fraction of the isolated plasma was utilized at the discretion of clinical necessity for routine serological analysis, including measurements of clinical biomarkers of inflammation: CRP, IL-6, and PCT. Following the analysis, any residual plasma was initially stored at 4°C, and subsequently relocated to a long-term storage facility at -80°C within 24h for biobanking purposes. Upon sample selection, specific samples were retrieved from the biobank and transported to the analytical chemistry laboratory on dry ice. Upon arrival, these samples were stored at -80°C until aliquoting for metabolomic analysis.

S2. Metabolomic Data Acquisition

S2.1 Amines

Amino acids and biogenic amines in plasma were profiled using ultra performance liquid chromatography tandem mass spectrometry (UPLC-MS/MS), following a method adapted from Noga *et al.*¹ This approach involved derivatization using the AccQ-TagTM Ultra derivatization kit procured from Waters Corporation (Etten-Leur, the Netherlands). Plasma samples (5 μL) were prepared by spiking with an internal standard solution (30 μL) composed of a mix of ¹³C¹⁵N-labeled amino acid analogs. Protein precipitation was achieved by the addition of 75 μL of MeOH, following which samples were centrifuged to isolate and dry the resulting supernatant in a SpeedVac. The residue was reconstituted in 80 μL of the borate buffer (pH 8.8) with 20 μL of AQC reagent for derivatization. After derivatization,

samples were heated for 30 min at 55°C at a speed of 900 rpm on an incubating microplate shaker, following which they were transferred to autosampler vials and cooled to 4°C until injection into the UPLC-MS/MS system. An Agilent 1290 Infinity II System equipped with a Waters AccQ-Tag Ultra C18 column (2.1 × 100 mm, 1.7 μm) was used for the chromatographic separation of analytes from an injection volume of 1 μL. Targets were detected and measured in the positive electrospray ionization (ESI) mode using multiple reaction monitoring (MRM) with nominal mass resolution in an AB Sciex QTRAP 6500 triple-quadrupole MS. Peak integration of the acquired MRM data was performed using the vendor software Sciex MultiQuant (v3.0.2).

S2.2 Signaling Lipids

Lipids involved in signaling pathways were measured in plasma using reversed-phase UHPLC-MS/MS, adapting the protocol published by Yang *et al.*,² which employed two chromatographic methods to cover a wide range of compound classes; a low pH method for various oxylipins (such as prostaglandins and isoprostanes), endocannabinoids, and bile acids, and a high pH method for lysosphingolipids, lysoglycerophospholipids, and fatty acids ranging from C14 to C22 chain length species. Sample preparation involved spiking plasma samples (50 μL) with 5 μL of antioxidant solution (0.2 mg mL⁻¹ BHT and 0.2 mg mL⁻¹ EDTA), 5 μL of internal standard solution composed of deuterated target compounds, and 50 μL of 0.2 M citric acid and 0.4 M disodium hydrogen phosphate buffer (pH 4.5). Lipid extraction was performed using 400 μL of Butanol:MTBE (1:1 v/v) liquid-liquid extraction method. 350 μL of resulting organic phase was isolated, concentrated by drying in a SpeedVac, and reconstituted in a 50 μL of 70:30 (v/v) mixture of methanol and acetonitrile (MeOH:ACN) before transfer to autosampler vials for injection into the UPLC-MS/MS system. For chromatographic separation, a Shimadzu LC formed by three high pressure pumps (LC-30AD), communication module (CBM-20A), autosampler (SIL-30AC), and an oven (CTO-30A) from Shimadzu Benelux was utilized, employing a Waters BEH C18 column (2.1 × 50 mm, 1.7 μm) for the low pH analysis (10 μL injection volume) and a Kinetex EVO C18 column (2.1 × 50 mm, 1.7 μm) for the high pH analysis (5 μL injection volume). ESI-MS was conducted using a Sciex QTRAP 7500 triple-quadrupole MS for low pH analysis and a Sciex QTRAP 6500+ MS for high pH analysis, with polarity switching and dynamic MRM. Peak integration of the acquired MRM data was performed using the vendor software Sciex OS (v2.1.6.59781).

S3. Data Preprocessing

Quality control was conducted with an in-house software using pooled study samples, method blanks, and internal standards. Peak area ratios were computed using the closest

eluting internal standard to correct for variations in sample preparation and instrument response. Metabolites with a relative standard deviation <30% in quality control samples prepared by pooling study samples and background signal <40% in method blanks were included for downstream analysis, resulting in 254 of the 317 measured targets. Metabolites with missing data were examined using Fisher's exact test to assess whether missingness was associated with specific groups, and metabolites exceeding 20% missingness were excluded. Additionally, 66 biologically pertinent metabolite ratios and 16 sums (or means) were computed to provide insights into enzyme activities and shifts in metabolic pathways.

S4. Statistics

All descriptive statistics, statistical tests, and visualization were performed in RStudio (v4.3.1). Univariate differential analysis was performed on the comprehensive dataset using linear mixed-effect models (LMMs), via the lme4 package (version 1.1.34) with metabolite as the response, a dichotomous variable representing the comparison groups as the predictor, and patient identifier as random effects ($1 \mid \text{patient identifier}$) to account for within-individual variability. The models were corrected for clinical confounders identified by Fisher's exact test for categorical variables, Welch's t-test for continuous variables, and visual inspection by Principal Component Analysis (PCA). LMMs were weighted by the inverse number of samples per patient to down weigh oversampled patients. P-values for the LMMs were obtained using the lmerTest package via the Satterthwaite's degrees of freedom method. Two primary models were implemented to elucidate the similarities and differences between SINS and sepsis. First, the SINS and sepsis cases were combined into the "Inflamed" group and compared with controls to identify systemic inflammation-associated traits independent of etiology. Second, the control and SINS cases were combined into the non-sepsis group and compared with the "Sepsis" group to isolate sepsis-specific signatures amid systemic inflammation-associated traits. Additionally, an ANOVA across the three groups was performed, complemented by LMMs of pairwise comparisons: (i) control versus SINS (C_SINS model), (ii) control versus sepsis (C_S model), and (iii) SINS versus sepsis (SINS_S model) to validate the results of the two larger models and ensure an accurate interpretation of metabolic alterations by determining group-driven associations. Additional analyses investigated the combination of control and SINS vs sepsis, i.e., the Sepsis model to datasets stratified by sex, pathogen, and blood culture result. LMM outcomes were visualized using volcano plots and compared using forest plots and directed p-value plots, where the directed p-values were obtained by multiplying the negative logarithm (base 10) of the p-value with the direction of the estimate. ANOVA was performed on log₂-transformed data prior adjusting for confounding factors, while mean fold change (FC) was

calculated on untransformed data and considered when exceeding the RSD-defined technical variation from pooled study samples.

Univariate logistic regression analyses were conducted using generalized linear models with a logit link function on the STP dataset to investigate the potential of metabolites as early diagnostic biomarkers for sepsis. The binary response variable represented the comparison groups (control vs. SINS, control vs. sepsis, SINS vs. sepsis), with metabolite as predictor adjusted for the confounders stated earlier. These models yield insights into the association between metabolite levels and the likelihood or log odds of belonging to a specific group. Subsequently, multivariable diagnostic metabolomic models were developed to distinguish between SINS and sepsis at the timepoint of sepsis suspicion. A bootstrap-aggregated LASSO logistic regression, with 100 bootstrap iterations, was employed to mitigate overfitting and reduce the risk of data leakage given the limited sample size ($n=57$). In each iteration, samples were drawn with replacement to form the training set, while the remaining out-of-bag samples served as an internal test set. LASSO regression was performed within the training set via the *glmnet* package (version 4.1.8) with the *cv.glmnet* function, incorporating a 10-fold cross-validation to optimize the regularization parameter (λ). Model performance was evaluated on out-of-bag test samples, and metrics including area under the curve (AUC), sensitivity, and specificity were averaged across all iterations to estimate overall predictive performance. Robust features were identified by calculating the frequency of variable selection across all bootstraps. Metabolites selected in $>45\%$ of bootstrap models were retained to build a reduced, targeted logistic regression model. This final metabolomic model was evaluated using Leave-One-Out-Cross-Validation, thereby deriving the Area Under the Receiving Operating Characteristics Curve (AUROC) to assess the predictive performance parameters of the model. Additional models incorporating individual routine clinical inflammatory markers, combinations of the inflammatory markers, and combinations of the inflammatory markers and metabolites were assessed to compare the metabolomic model to conventional clinical diagnostic practices for sepsis detection. The McNemar's test was applied to the paired predictions from the reduced metabolite-based and inflammatory marker models to assess statistically significant differences in classification performance. Additionally, spearman correlations were calculated between diagnostic panel metabolites and inflammatory markers to provide complementary information. To further understand how these relationships shift under different inflammatory conditions, differential correlations were computed using the *compcorr* function from the DiffCorr package. A significance threshold of 0.05 was applied to p-values across all statistical analyses. To account for multiple testing, p-values were adjusted using Benjamini-Hochberg method implemented by the *p.adjust* function. These adjusted p-values, termed q-values, were

subjected to a significance threshold of 0.1. These corrections accounted for the total number of metabolic features in univariate tests (n=296).

S5. Univariate Logistic Regression Model Results

Univariate analysis assessing the diagnostic utility of metabolites by determining the strength and direction of association between metabolites and odds of the condition, identified 61 metabolites with $p < 0.05$ in the C_S model, of which 26 retained statistical significance after multiple testing correction ($q < 0.1$). No statistically significant metabolites were observed in the C_SINS and SINS_S models, potentially due to reduced sample size within the STP dataset. However, 47 metabolites in the C_SINS model and 14 metabolites in the SINS_S model showed potential diagnostic utility ($p < 0.05$; $q > 0.1$). A comparison between the C_S and C_SINS models revealed that 31 of the 61 metabolites were exclusively associated with sepsis (**Figure S5a**). Several of these metabolites were also identified as differentially regulated in sepsis in the univariate analysis. Notably, phenylalanine/tyrosine (log OR: 4.46; 95% CI: 2.37-7.57), BCAA/AAA (log OR: 4.06; 95% CI: 1.69-7.03), LPE(16:0) (log OR: 3.25; 95% CI: 1.40-5.63), and LPI(16:0) (log OR: 4.17; 95% CI: 2.05-7.28), were associated with higher odds of sepsis, while 3-methoxy-tyrosine (log OR: -1.75; 95% CI: -3.22- -0.53), citrulline (log OR: -1.88; 95% CI: -3.51- -0.57), glutamine/glutamate (log OR: -1.20; 95% CI: -2.23- -0.31), 4-hydroxyproline/proline (log OR: -2.92; 95% CI: -5.18- -1.10), and sum of OG (log OR: -1.20; 95% CI: -2.30- -0.30) were associated with lower odds of sepsis, when compared to control. Furthermore, analysis of the SINS_S model revealed metabolites such as cortisol (log OR: 1.08; 95% CI: 0.15-2.35), putrescine (log OR: 1.60; 95% CI: 0.36-3.32), 11beta-PGF2alpha/AA (log OR: 0.91; 95% CI: 0.16-1.85), S1P(18 :2) (log OR: -2.41; 95% CI: -5.17- -0.28), and LPA(20.4) (log OR: -1.70; 95% CI: -3.56- -0.22) as potential biomarkers for distinguishing between SINS and sepsis (**Figure S5b**). Details of these logistic regression models are documented in **Tables S12-S14**.

Supplementary References

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Supplementary Figures



Figure S1. Temporal distribution of samples in the comprehensive and single time point datasets. Samples from each patient are plotted against the postnatal age at the time of sampling, with colors and shapes representing different groups: control (*green; filled circle*), systemic inflammation-no sepsis (*light blue; filled square*), sepsis (*blue; square with a cross*), and follow up (*filled triangle*). The single time point dataset was curated by selecting one sample per patient, prioritizing sepsis samples, followed by systemic inflammation-no sepsis, and including first episodes in multi-episode cases. All matched controls from patients without sepsis or systemic inflammation-no sepsis were also included. The selected single time point samples are highlighted in *gold*.

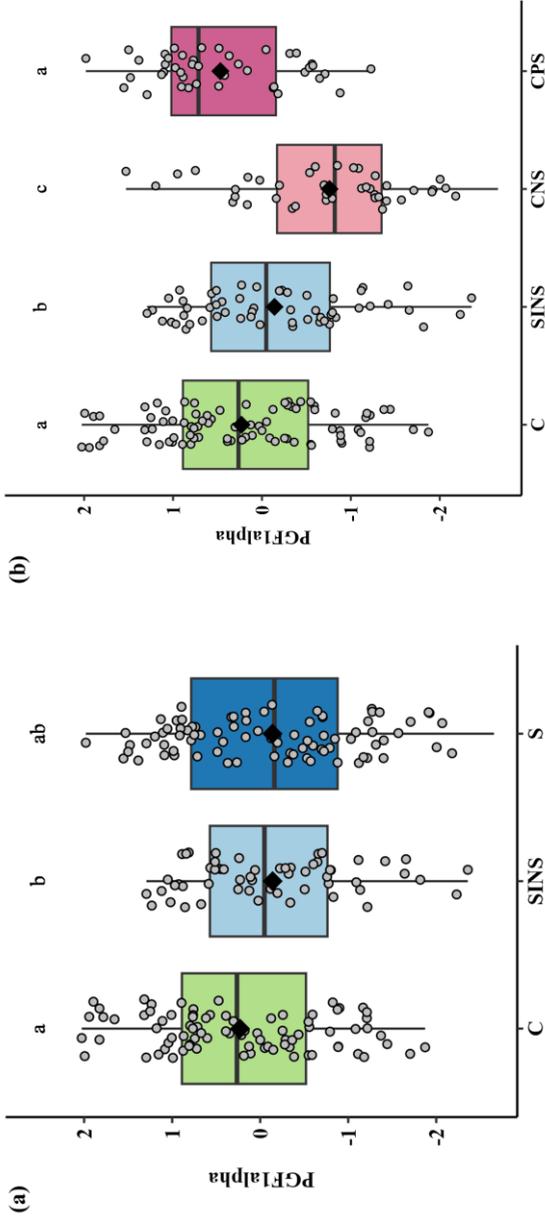


Figure S3. Differential regulation of PGF1alpha across SINS and sepsis subgroups. The figure presents a series of boxplots illustrating the distribution of PGF1alpha levels prior to confounder correction. (a) Boxplots illustrating the significant downregulation of PGF1alpha exclusively in the SINS group compared to controls, showing its distinct regulation in systemic inflammation without sepsis. (b) Boxplots depicting the stratification of the sepsis group by blood culture outcome, revealing contrasting patterns of PGF1alpha regulation, with significant downregulation in culture-negative sepsis and an upward trend in culture-positive sepsis. In each boxplot, the central line represents the mean, with box edges denoting the interquartile range. Individual data points represent samples, and the black diamond represents the mean. The letters denote significance between groups from the linear-mixed effect models: SINS = Systemic Inflammation-No Sepsis (*light blue*); S = Sepsis (*blue*); CNS = Culture-Negative Sepsis (*light pink*); CPS = Culture-Positive Sepsis (*dark pink*).

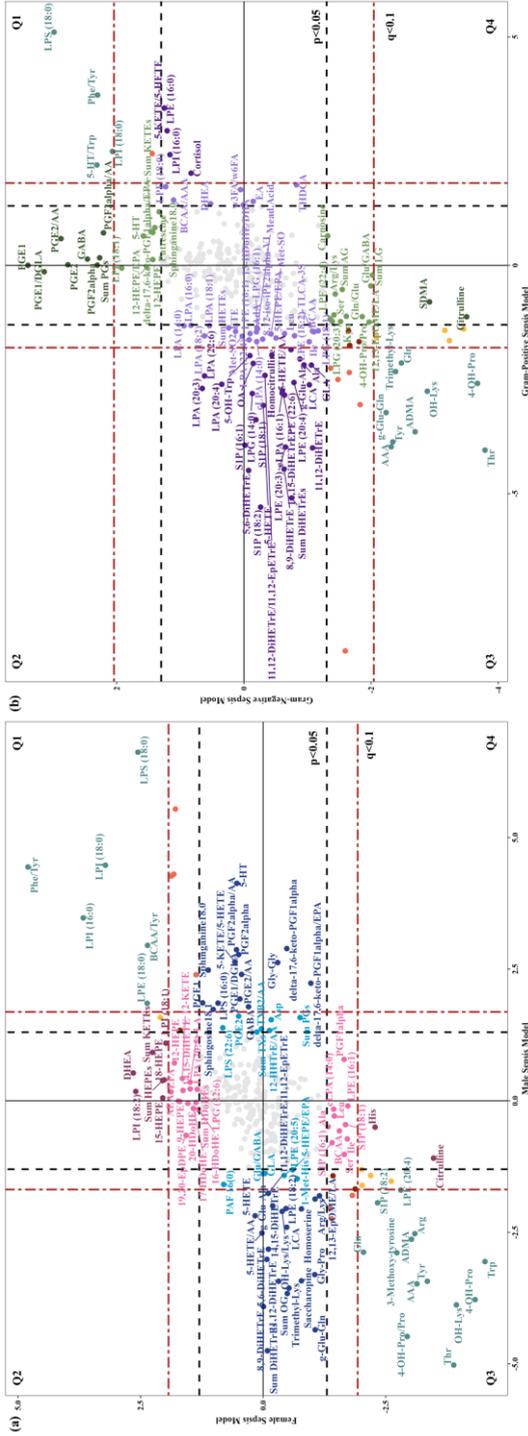


Figure S4. Comparative analysis of differentially regulated metabolites in sex- and pathogen-stratified linear mixed-effect sepsis models. The figure presents the directed p-value plots of the sex and pathogen-stratified analysis. The left panel (a) showcases the sex-stratified analysis, plotting the directed p-values of the male sepsis model in the x-axis and the directed p-values of the female sepsis model on the y-axis, color-coded based on significance level, before and after FDR correction (*dark pink*: significant after correction exclusively in female; *light pink*: significant before correction exclusively in female; *dark blue*: significant after correction exclusively in male; *light blue*: significant before correction exclusively in male; *slate gray*: significant after correction both in male and female). Metabolites in Q1 are increased in both males and females, those in Q2 are decreased in males and increased in females, those in Q3 are decreased in both males and females, and those in Q4 are increased in males and decreased in females. The right panel (b) displays the pathogen-stratified analysis, plotting the directed p-values of the gram-positive sepsis model in the x-axis and the directed p-values of the gram-negative sepsis model on the y-axis, color-coded based on significance level, before and after FDR correction (*dark purple*: significant after correction exclusively in gram-negative; *light purple*: significant before correction exclusively in gram-positive; *dark green*: significant after correction exclusively in gram-negative; *light green*: significant before correction exclusively in gram-positive; *slate gray*: significant after correction both in gram-negative and gram-positive). Metabolites in Q1 are increased in both gram-positive and gram-negative sepsis, those in Q2 are decreased in gram-positive and increased in gram-negative sepsis, those in Q3 are decreased in both gram-positive and gram-negative sepsis, and those in Q4 are increased in gram-positive and decreased in gram-negative sepsis. FDR = False Discovery Rate; Q = Quadrant.

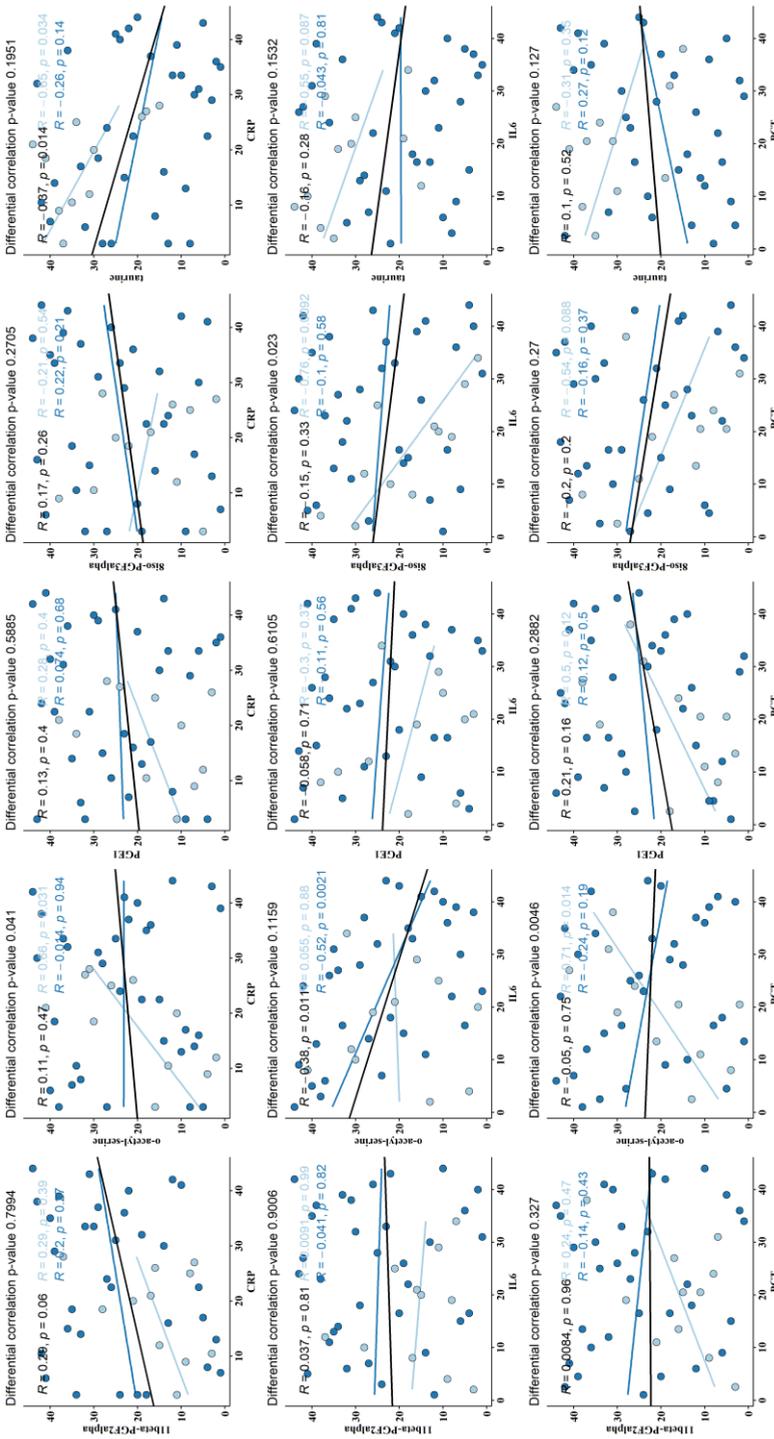


Figure S6. Spearman correlation analyses of the metabolites in the diagnostic panel with the ranks of the three routine inflammatory markers. The figure presents the scatter plots of the ranks of five metabolites in the diagnostic panel with the ranks of the three routine inflammatory markers. Each plot illustrates the correlation coefficient rho and p-value for all datapoints combined, as well as stratified by group (systemic inflammation-no sepsis (*light blue*) and sepsis (*dark blue*)). The differential correlation p-value is also displayed in each plot to highlight significant differences between the two groups. BCAA: Branched Chain Amino Acids; AAA: Aromatic Amino Acids.

Supplementary Tables

Table S1: Missing data patterns of metabolites exhibiting greater than 20% missingness

Metabolite	Overall Missing Percentage	Missing Percentage in Non-Sepsis Group	Missing Percentage in Sepsis Group	Fisher's exact test p-value
iPF2a-IV	56.6	66.67	40.66	0.0014
GUDCA	83.83	89.58	74.73	0.0035
6-keto-PGF1a	41.7	49.31	29.67	0.0042
ResolvinE1	85.11	90.28	76.92	0.0078
13,14-dihydro-PGF2a	88.51	84.72	94.51	0.022
NO2-OA	77.02	72.22	84.62	0.038
1a,1b-dihomo-PGF2a	80.85	76.39	87.91	0.04
20-carboxy-LTB4	42.13	47.22	34.07	0.058
UDCA	77.02	81.25	70.33	0.058
PGE3	88.51	91.67	83.52	0.062
14,15-EpETE	96.17	97.92	93.41	0.093
15deoxy-12,14-PGD2	61.28	56.94	68.13	0.1
4-HDoHE	29.79	33.33	24.18	0.15
8iso-PGA2	23.4	20.14	28.57	0.16
11beta-PGE2	88.09	90.28	84.62	0.22
LTB5	69.36	72.22	64.84	0.25
8iso-PGA1	21.28	18.75	25.27	0.25
8iso-PGE1	84.68	86.81	81.32	0.27
CDCA	58.3	61.11	53.85	0.28
2,3dinor-11beta-PGF2a	53.19	56.25	48.35	0.28
GLCA	27.23	29.86	23.08	0.29
9-HETE	37.45	34.72	41.76	0.33
GDCA	94.04	95.14	92.31	0.41
Maresin1	93.19	94.44	91.21	0.43
5,15-DiHETE	90.21	88.89	92.31	0.5
16,17-EpDPE	71.06	72.22	69.23	0.66
TLCA	82.13	81.25	83.52	0.73
8,9-EpETrE	20.43	19.44	21.98	0.74
HDCA	75.32	74.31	76.92	0.76
10,17-DiHDoHE	70.64	71.53	69.23	0.77
NADA	94.47	93.75	95.6	0.77
12,13-DiHODE	45.11	45.83	43.96	0.79
PGJ2	90.64	90.97	90.11	0.82
ResolvinD5	85.96	85.42	86.81	0.85
8iso-PGF2a	65.53	65.97	64.84	0.89
6trans-LTB4	34.89	34.72	35.16	1
9,10-DiHOME	31.06	31.25	30.77	1
10-NO2-LA	76.17	76.39	75.82	1
14,15-EpETrE	70.21	70.14	70.33	1
15deoxy-delta-12,14-PGJ2	26.81	27.08	26.37	1

Table S2: Linear mixed-effect model results of the "Inflamed" model comparing control with inflamed groups

Metabolite	Category	Estimate	Standard Error	z-value	p-value	Adjusted p-value
LPS (18:0)	Lysophospholipid	0.8998	0.1246	7.2203	1.4513E-11	4.2959E-09
Trp	Amine	-0.6721	0.1069	-6.2863	2.1805E-09	3.2271E-07
Gln	Amine	-0.7647	0.1344	-5.6885	4.3678E-08	4.3096E-06
Cortisol	Steroid Hormone	0.7248	0.1297	5.5872	7.4948E-08	5.5462E-06
Thr	Amine	-0.6568	0.1191	-5.5165	1.0767E-07	6.3740E-06
g-Glu-Gln	Amine	-0.7369	0.1401	-5.2615	3.5556E-07	1.7541E-05
4-OH-Pro	Amine	-0.6453	0.1256	-5.1373	6.4046E-07	2.7082E-05
OH-Lys	Amine	-0.6532	0.1297	-5.0369	1.0086E-06	3.7317E-05
LPI (18:0)	Lysophospholipid	0.6169	0.1288	4.7912	3.1801E-06	1.0459E-04
Phe/Tyr	Amine	0.4299	0.0913	4.7073	4.5815E-06	1.3561E-04
5-HT/Trp	Amine	0.6540	0.1431	4.5693	8.3970E-06	2.2596E-04
Saccharopine	Amine	-0.6232	0.1428	-4.3633	2.0160E-05	4.7254E-04
His	Amine	-0.5509	0.1262	-4.3638	2.0754E-05	4.7254E-04
Arg	Amine	-0.5836	0.1372	-4.2540	3.1849E-05	6.7337E-04
ADMA	Amine	-0.5546	0.1335	-4.1541	4.8406E-05	9.2806E-04
Gln/Glu	Amine	-0.6118	0.1475	-4.1487	5.0273E-05	9.2806E-04
SIP (18:2)	Lysophospholipid	-0.4640	0.1126	-4.1225	5.4497E-05	9.2806E-04
4-OH-Pro/Pro	Amine	-0.5335	0.1298	-4.1113	5.6436E-05	9.2806E-04
8,9-DiHETrE	Oxylipin	-0.5442	0.1341	-4.0566	6.9722E-05	1.0370E-03

Diagnosis of Late-Onset Sepsis

Sum DiHETrEs	Oxylipin	-0.5149	0.1269	-4.0577	7.0070E-05	1.0370E-03
Sum OG	Endocannabinoid	-0.5732	0.1420	-4.0371	7.6957E-05	1.0650E-03
LPE (16:0)	Lysophospholipid	0.4893	0.1218	4.0182	8.1753E-05	1.0650E-03
Lys	Amine	-0.5256	0.1309	-4.0150	8.2750E-05	1.0650E-03
cLPA (16:1)	Lysophospholipid	-0.5321	0.1334	-3.9888	9.1057E-05	1.1230E-03
LCA	Bile Acid	-0.5229	0.1321	-3.9590	1.0533E-04	1.2471E-03
Ornithine	Amine	-0.4987	0.1291	-3.8617	1.5088E-04	1.7177E-03
LPE (22:6)	Lysophospholipid	-0.5175	0.1369	-3.7790	2.0687E-04	2.2679E-03
LPI (16:0)	Lysophospholipid	0.5239	0.1398	3.7486	2.2923E-04	2.4233E-03
Met	Amine	-0.5086	0.1366	-3.7233	2.5259E-04	2.5781E-03
Ser	Amine	-0.5034	0.1362	-3.6954	2.8704E-04	2.8321E-03
AAA	Amine	-0.4409	0.1202	-3.6680	3.1370E-04	2.9953E-03
Tyr	Amine	-0.3913	0.1081	-3.6213	3.6909E-04	3.3398E-03
LPE (22:4)	Lysophospholipid	-0.4213	0.1165	-3.6166	3.7234E-04	3.3398E-03
LPE (20:4)	Lysophospholipid	-0.4391	0.1231	-3.5666	4.4851E-04	3.9047E-03
5,6-DiHETrE	Oxylipin	-0.4394	0.1243	-3.5347	5.0142E-04	4.2406E-03
LPE (20:3)	Lysophospholipid	-0.4396	0.1260	-3.4879	5.9191E-04	4.8668E-03
Gly	Amine	-0.4274	0.1254	-3.4091	7.8670E-04	6.2936E-03
S-Methyl-Cys	Amine	-0.4434	0.1325	-3.3450	9.7097E-04	7.5633E-03
11,12-DiHETrE	Oxylipin	-0.4150	0.1275	-3.2542	1.3214E-03	1.0029E-02
Gly-Pro	Amine	-0.3885	0.1221	-3.1827	1.6883E-03	1.2493E-02
PGE2/AA	Oxylipin	0.4468	0.1445	3.0929	2.2560E-03	1.6287E-02
Ile	Amine	-0.4675	0.1524	-3.0673	2.4535E-03	1.7292E-02
cLPA (14:0)	Lysophospholipid	-0.3005	0.0987	-3.0454	2.6151E-03	1.8001E-02
Citrulline	Amine	-0.3608	0.1196	-3.0162	2.8699E-03	1.9307E-02
PGF1alpha	Oxylipin	-0.3149	0.1047	-3.0082	2.9415E-03	1.9348E-02
5-HT	Amine	0.4242	0.1447	2.9313	3.7564E-03	2.4172E-02
Asn	Amine	-0.3101	0.1063	-2.9164	3.9759E-03	2.4644E-02
SDMA	Amine	-0.3499	0.1202	-2.9099	3.9963E-03	2.4644E-02
DEA	Endocannabinoid	0.4056	0.1444	2.8084	5.4880E-03	3.2724E-02
BCAA	Amine	-0.4058	0.1447	-2.8050	5.5278E-03	3.2724E-02
5-HETE/AA	Oxylipin	-0.3527	0.1273	-2.7708	6.1049E-03	3.5433E-02
5-KETE/5-HETE	Oxylipin	0.3605	0.1305	2.7620	6.3807E-03	3.6321E-02
LPE (18:2)	Lysophospholipid	-0.3354	0.1248	-2.6885	7.7407E-03	4.3231E-02
PGE1	Oxylipin	0.4081	0.1523	2.6787	7.9967E-03	4.3834E-02
PGE1/DGLA	Oxylipin	0.4004	0.1514	2.6454	8.7891E-03	4.7302E-02
SIP (18:1)	Lysophospholipid	-0.3136	0.1198	-2.6181	9.5163E-03	4.9554E-02
PGE2	Oxylipin	0.3982	0.1522	2.6163	9.5425E-03	4.9554E-02
3-Methoxy-tyrosine	Amine	-0.3468	0.1333	-2.6015	9.9279E-03	5.0667E-02
Sum HEPeEs	Oxylipin	0.3324	0.1290	2.5768	1.0656E-02	5.2334E-02
9-KODE/9-HODE	Oxylipin	-0.3349	0.1299	-2.5774	1.0659E-02	5.2334E-02
Sum SBA	Bile Acid	-0.4045	0.1572	-2.5730	1.0785E-02	5.2334E-02
18-HEPE	Oxylipin	0.3277	0.1280	2.5604	1.1210E-02	5.3520E-02
LPE (20:5)	Lysophospholipid	-0.3386	0.1332	-2.5409	1.1764E-02	5.4871E-02
PGF2alpha	Oxylipin	0.3888	0.1533	2.5359	1.1933E-02	5.4871E-02
14,15-DiHETrE	Oxylipin	-0.3266	0.1290	-2.5318	1.2079E-02	5.4871E-02
LPE (18:0)	Lysophospholipid	0.2910	0.1151	2.5275	1.2235E-02	5.4871E-02
Val	Amine	-0.3349	0.1349	-2.4819	1.3884E-02	6.1338E-02
TLCA-3S	Bile Acid	-0.3558	0.1459	-2.4392	1.5531E-02	6.6864E-02
DHEA	Endocannabinoid	0.1999	0.0820	2.4382	1.5587E-02	6.6864E-02
Leu	Amine	-0.3602	0.1498	-2.4048	1.7115E-02	7.2370E-02
LPS (16:0)	Lysophospholipid	0.3442	0.1447	2.3783	1.8289E-02	7.6249E-02
Homoserine	Amine	-0.3241	0.1373	-2.3603	1.9171E-02	7.8815E-02
Trimethyl-Lys	Amine	-0.3043	0.1301	-2.3400	2.0227E-02	8.1406E-02
LPS (18:2)	Lysophospholipid	0.2963	0.1267	2.3389	2.0351E-02	8.1406E-02
PGF2alpha/AA	Oxylipin	0.3362	0.1447	2.3230	2.1123E-02	8.3364E-02
14-HDoHE/DHA	Oxylipin	0.3306	0.1428	2.3157	2.1613E-02	8.4176E-02
Ala	Amine	-0.3254	0.1413	-2.3033	2.2232E-02	8.4856E-02
LPS (18:1)	Lysophospholipid	0.3444	0.1499	2.2970	2.2655E-02	8.4856E-02
SIP (16:1)	Lysophospholipid	-0.2329	0.1015	-2.2955	2.2723E-02	8.4856E-02
LPS (22:4)	Lysophospholipid	0.3342	0.1459	2.2912	2.2934E-02	8.4856E-02
Arg/Lys	Amine	-0.3285	0.1447	-2.2699	2.4323E-02	8.8882E-02
BCAA/Tyr	Amine	0.2145	0.0950	2.2579	2.4989E-02	9.0205E-02
LPI (18:1)	Lysophospholipid	0.3043	0.1365	2.2300	2.6848E-02	9.5747E-02
Sum KETEs	Oxylipin	0.3180	0.1434	2.2170	2.7674E-02	9.7516E-02
12-HEPE	Oxylipin	0.2895	0.1318	2.1972	2.9126E-02	1.0143E-01
LPE (16:1)	Lysophospholipid	-0.2910	0.1327	-2.1935	2.9556E-02	1.0173E-01
5-HETE	Oxylipin	-0.3197	0.1477	-2.1649	3.1541E-02	1.0731E-01
12,13-EpOME/LA	Oxylipin	-0.2756	0.1324	-2.0816	3.8574E-02	1.2975E-01
Cys	Amine	-0.2665	0.1296	-2.0566	4.0957E-02	1.3622E-01
Kyn	Amine	-0.2792	0.1398	-1.9975	4.7085E-02	1.5486E-01
LPS (22:6)	Lysophospholipid	0.2105	0.1061	1.9843	4.8506E-02	1.5778E-01
EA	Amine	0.2364	0.1206	1.9609	5.1199E-02	1.6473E-01
9-HODE/9-HpODE	Oxylipin	0.2649	0.1385	1.9120	5.7289E-02	1.8104E-01

Chapter III

Cystathionine	Amine	-0.2126	0.1115	-1.9058	5.8067E-02	1.8104E-01
Met-SO2	Amine	-0.2151	0.1130	-1.9033	5.8381E-02	1.8104E-01
GLA	Fatty acid	-0.2634	0.1388	-1.8985	5.9014E-02	1.8104E-01
1-Met-His	Amine	-0.2590	0.1367	-1.8941	5.9557E-02	1.8104E-01
11,12-EpETrE/AA	Oxylipin	-0.2596	0.1373	-1.8908	6.0041E-02	1.8104E-01
5-HEPE/EPA	Oxylipin	-0.1737	0.0921	-1.8870	6.0550E-02	1.8104E-01
Sum LG	Endocannabinoid	-0.2255	0.1202	-1.8765	6.1994E-02	1.8350E-01
OA	Fatty acid	-0.2732	0.1476	-1.8512	6.5579E-02	1.9219E-01
Sphingosine 18.1	Lysophospholipid	0.2733	0.1497	1.8265	6.9216E-02	2.0086E-01
14-HDoHE	Oxylipin	0.2772	0.1541	1.7982	7.3747E-02	2.1193E-01
Arg/ADMA	Amine	-0.2642	0.1480	-1.7852	7.5747E-02	2.1559E-01
Carnosine	Amine	-0.2044	0.1155	-1.7690	7.8328E-02	2.2081E-01
Anserine	Amine	-0.2509	0.1424	-1.7620	7.9618E-02	2.2124E-01
12-HETE/AA	Oxylipin	0.2650	0.1511	1.7542	8.0911E-02	2.2124E-01
12-HHTrE	Oxylipin	0.2190	0.1250	1.7518	8.1286E-02	2.2124E-01
11,12-EpETrE	Oxylipin	-0.2156	0.1232	-1.7505	8.1469E-02	2.2124E-01
9-HpODE/LA	Oxylipin	-0.2420	0.1387	-1.7448	8.2445E-02	2.2185E-01
18-HEPE/EPA	Oxylipin	0.2340	0.1346	1.7376	8.3849E-02	2.2331E-01
PGF1alpha/DGLA	Oxylipin	-0.2085	0.1205	-1.7299	8.5130E-02	2.2331E-01
8-HETrE/DGLA	Oxylipin	0.2513	0.1453	1.7293	8.5250E-02	2.2331E-01
12-KETE	Oxylipin	0.2411	0.1399	1.7226	8.6401E-02	2.2434E-01
Sum TXs		0.2366	0.1380	1.7148	8.7856E-02	2.2613E-01
Sum AG	Endocannabinoid	-0.2309	0.1355	-1.7037	8.9918E-02	2.2945E-01
Kyn/Trp	Amine	0.2453	0.1459	1.6816	9.4157E-02	2.3821E-01
g-Glu-Ala	Amine	-0.2249	0.1345	-1.6730	9.5805E-02	2.4035E-01
HomoCys	Amine	-0.2301	0.1391	-1.6547	9.9442E-02	2.4657E-01
11-HDoHE/DHA	Oxylipin	0.2466	0.1492	1.6526	9.9959E-02	2.4657E-01
LPG (14:0)	Lysophospholipid	-0.1587	0.0966	-1.6434	1.0177E-01	2.4737E-01
LPA (20:5)	Lysophospholipid	0.2049	0.1248	1.6420	1.0210E-01	2.4737E-01
Sarcosine	Amine	-0.2259	0.1379	-1.6384	1.0279E-01	2.4737E-01
beta-Ala	Amine	-0.2126	0.1314	-1.6186	1.0701E-01	2.5153E-01
12-HHTrE/AA	Oxylipin	0.1977	0.1223	1.6159	1.0770E-01	2.5153E-01
LPG (20:3)	Lysophospholipid	-0.2372	0.1472	-1.6116	1.0853E-01	2.5153E-01
TXB2	Oxylipin	0.2124	0.1318	1.6109	1.0870E-01	2.5153E-01
11,12-DiHETrE/11,12-EpETrE	Oxylipin	-0.2042	0.1268	-1.6105	1.0877E-01	2.5153E-01
cLPA (18:2)	Lysophospholipid	-0.2007	0.1258	-1.5954	1.1213E-01	2.5729E-01
12-HEPE/EPA	Oxylipin	0.2281	0.1436	1.5880	1.1386E-01	2.5873E-01
Gly-Gly	Amine	0.2000	0.1261	1.5861	1.1451E-01	2.5873E-01
20-HDoHE/DHA	Oxylipin	0.2206	0.1397	1.5784	1.1598E-01	2.6007E-01
Sphinganine 18.0	Lysophospholipid	0.2335	0.1495	1.5617	1.1989E-01	2.6451E-01
LPG (20:4)	Lysophospholipid	-0.1910	0.1224	-1.5604	1.2016E-01	2.6451E-01
TXB2/AA	Oxylipin	0.2020	0.1296	1.5587	1.2064E-01	2.6451E-01
O-PO3-EA	Amine	0.2341	0.1512	1.5485	1.2313E-01	2.6799E-01
12-HETE	Oxylipin	0.2331	0.1535	1.5186	1.3044E-01	2.7940E-01
cLPA (20:4)	Lysophospholipid	-0.2004	0.1322	-1.5160	1.3104E-01	2.7940E-01
EPA	Fatty acid	0.1254	0.0828	1.5152	1.3120E-01	2.7940E-01
Tau	Amine	0.1981	0.1316	1.5045	1.3391E-01	2.8152E-01
LPE (22:5)	Lysophospholipid	-0.2057	0.1368	-1.5038	1.3410E-01	2.8152E-01
Putrescine	Amine	0.2034	0.1362	1.4933	1.3684E-01	2.8524E-01
15-HETrE/DGLA	Oxylipin	0.2236	0.1503	1.4878	1.3831E-01	2.8629E-01
O-Acetyl-Ser	Amine	-0.1929	0.1311	-1.4710	1.4277E-01	2.9179E-01
GCA	Bile Acid	-0.2152	0.1467	-1.4676	1.4369E-01	2.9179E-01
Pro	Amine	-0.2106	0.1435	-1.4672	1.4392E-01	2.9179E-01
LPG (16:1)	Lysophospholipid	-0.2124	0.1459	-1.4563	1.4683E-01	2.9566E-01
DPA	Fatty acid	-0.2039	0.1406	-1.4500	1.4855E-01	2.9710E-01
ALA	Fatty acid	0.1400	0.0981	1.4276	1.5486E-01	3.0721E-01
8-iso-PGF3alpha	Oxylipin	-0.1415	0.0993	-1.4260	1.5568E-01	3.0721E-01
5-HETrE	Oxylipin	-0.1833	0.1329	-1.3793	1.6929E-01	3.3186E-01
TXB1	Oxylipin	0.1890	0.1380	1.3695	1.7228E-01	3.3343E-01
FA (16:0)	Fatty acid	-0.2034	0.1485	-1.3697	1.7235E-01	3.3343E-01
LA	Fatty acid	0.1411	0.1037	1.3604	1.7514E-01	3.3664E-01
15-HEPE	Oxylipin	0.1592	0.1176	1.3539	1.7725E-01	3.3849E-01
Sum HD0HEs	Oxylipin	0.1943	0.1464	1.3267	1.8616E-01	3.5323E-01
PGA2	Oxylipin	0.1827	0.1385	1.3191	1.8857E-01	3.5448E-01
TCA	Bile Acid	-0.1558	0.1183	-1.3174	1.8922E-01	3.5448E-01
CA	Bile Acid	0.1749	0.1356	1.2898	1.9851E-01	3.6955E-01
LPG (18:1)	Lysophospholipid	-0.1877	0.1470	-1.2771	2.0295E-01	3.7429E-01
8-iso-PGF3alpha/DGLA	Oxylipin	-0.1446	0.1133	-1.2758	2.0358E-01	3.7429E-01
TXB1/DGLA	Oxylipin	0.1716	0.1388	1.2365	2.1768E-01	3.9774E-01
PAF 16(0)	PAF	-0.1849	0.1510	-1.2246	2.2207E-01	4.0283E-01
PGA2/AA	Oxylipin	0.1639	0.1342	1.2217	2.2319E-01	4.0283E-01
10-HDoHE/DHA	Oxylipin	0.1769	0.1463	1.2094	2.2795E-01	4.0839E-01
OH-Lys/Lys	Amine	-0.1584	0.1313	-1.2063	2.2903E-01	4.0839E-01
9-HEPE	Oxylipin	0.1337	0.1118	1.1956	2.3324E-01	4.1341E-01

Diagnosis of Late-Onset Sepsis

20-HDoHE	Oxylipin	0.1586	0.1331	1.1912	2.3489E-01	4.1385E-01
12,13-EpOME	Oxylipin	-0.1650	0.1395	-1.1831	2.3809E-01	4.1700E-01
cLPA (18:1)	Lysophospholipid	-0.1487	0.1263	-1.1779	2.4019E-01	4.1821E-01
AdA	Fatty acid	-0.1663	0.1428	-1.1648	2.4540E-01	4.2479E-01
LPI (22:4)	Lysophospholipid	-0.1527	0.1315	-1.1609	2.4700E-01	4.2506E-01
LPG (18:2)	Lysophospholipid	-0.1380	0.1209	-1.1416	2.5492E-01	4.3617E-01
3-Met-His	Amine	0.1661	0.1469	1.1309	2.5937E-01	4.4114E-01
AEA	Endocannabinoid	0.1223	0.1084	1.1278	2.6081E-01	4.4114E-01
11-HDoHE	Oxylipin	0.1547	0.1381	1.1204	2.6387E-01	4.4379E-01
13-HDoHE/DHA	Oxylipin	0.1649	0.1487	1.1086	2.6886E-01	4.4962E-01
17-HDoHE/DHA	Oxylipin	0.1655	0.1502	1.1018	2.7183E-01	4.5163E-01
GABA	Amine	0.1623	0.1477	1.0988	2.7311E-01	4.5163E-01
5-iPF2alpha-VI/AA	Oxylipin	0.1527	0.1405	1.0871	2.7835E-01	4.5773E-01
Asp	Amine	0.1556	0.1442	1.0788	2.8206E-01	4.6127E-01
9-HpODE	Oxylipin	-0.1280	0.1257	-1.0183	3.0967E-01	5.0364E-01
LPE (18:1)	Lysophospholipid	-0.1210	0.1227	-0.9866	3.2495E-01	5.2560E-01
BCAA/AAA	Amine	0.1008	0.1040	0.9691	3.3358E-01	5.3663E-01
Ornithine/Arg	Amine	0.1431	0.1533	0.9339	3.5149E-01	5.6239E-01
5-iPF2alpha-VI	Oxylipin	0.1291	0.1389	0.9294	3.5374E-01	5.6294E-01
LPI (18:2)	Lysophospholipid	0.1018	0.1101	0.9244	3.5633E-01	5.6403E-01
11beta-PGF2alpha/AA	Oxylipin	-0.1052	0.1146	-0.9183	3.5967E-01	5.6629E-01
Mead.Acid	Fatty acid	-0.1220	0.1397	-0.8734	3.8348E-01	6.0059E-01
Met-SO	Amine	-0.1247	0.1439	-0.8663	3.8729E-01	6.0335E-01
11-HETE	Oxylipin	0.1216	0.1459	0.8332	4.0564E-01	6.2863E-01
12,13-DiHOME/12,13-EpOME	Oxylipin	0.0782	0.0946	0.8267	4.0936E-01	6.2907E-01
11beta-PGF2alpha	Oxylipin	-0.0756	0.0916	-0.8258	4.1017E-01	6.2907E-01
8-HETE	Oxylipin	0.1220	0.1488	0.8196	4.1341E-01	6.3077E-01
Citrulline/Ornithine	Amine	0.0934	0.1156	0.8078	4.2010E-01	6.3769E-01
5-HETrE/DGLA	Oxylipin	-0.1027	0.1280	-0.8020	4.2350E-01	6.3958E-01
9-HOTrE/ALA	Oxylipin	-0.0986	0.1271	-0.7756	4.3886E-01	6.5940E-01
8,12-iso-iPF2alpha-VI	Oxylipin	-0.1135	0.1488	-0.7630	4.4634E-01	6.6725E-01
10-HDoHE	Oxylipin	0.1038	0.1409	0.7366	4.6223E-01	6.8254E-01
THDCA	Bile Acid	0.0752	0.1022	0.7363	4.6236E-01	6.8254E-01
AABA	Amine	0.1066	0.1451	0.7344	4.6348E-01	6.8254E-01
delta-17,6-keto-PGF1alpha	Oxylipin	0.1024	0.1415	0.7240	4.6990E-01	6.8311E-01
Glu/GABA	Amine	-0.0973	0.1347	-0.7226	4.7075E-01	6.8311E-01
11-HETE/AA	Oxylipin	0.1075	0.1490	0.7217	4.7130E-01	6.8311E-01
13-HDoHE	Oxylipin	0.0851	0.1190	0.7157	4.7497E-01	6.8311E-01
8,12-iso-iPF2alpha-VI/AA	Oxylipin	-0.1010	0.1412	-0.7150	4.7541E-01	6.8311E-01
15-HETE/AA	Oxylipin	0.1028	0.1459	0.7047	4.8175E-01	6.8522E-01
17-HDoHE	Oxylipin	0.0911	0.1301	0.6999	4.8477E-01	6.8522E-01
DGLA	Fatty acid	-0.1040	0.1489	-0.6986	4.8556E-01	6.8522E-01
LPG (18:0)	Lysophospholipid	0.0897	0.1286	0.6977	4.8614E-01	6.8522E-01
9-KODE	Oxylipin	-0.0938	0.1352	-0.6938	4.8854E-01	6.8534E-01
LPG (22:6)	Lysophospholipid	0.0644	0.0937	0.6867	4.9303E-01	6.8657E-01
Phe	Amine	0.0957	0.1398	0.6846	4.9443E-01	6.8657E-01
GCDA	Bile Acid	-0.0786	0.1154	-0.6814	4.9637E-01	6.8657E-01
LPA (22:5)	Lysophospholipid	0.0905	0.1347	0.6718	5.0249E-01	6.9179E-01
7-HDoHE/DHA	Oxylipin	-0.0982	0.1473	-0.6669	5.0557E-01	6.9276E-01
LPA (14:0)	Lysophospholipid	0.0677	0.1021	0.6633	5.0787E-01	6.9276E-01
19,20-DiHDPA/19,20-EpDPE	Oxylipin	0.0887	0.1365	0.6503	5.1618E-01	6.9781E-01
TUDCA	Bile Acid	0.0913	0.1411	0.6471	5.1833E-01	6.9781E-01
12-KETE/12-HETE	Oxylipin	0.0963	0.1490	0.6465	5.1864E-01	6.9781E-01
15-HETrE	Oxylipin	0.0954	0.1488	0.6412	5.2210E-01	6.9928E-01
19,20-EpDPE/DHA	Oxylipin	-0.0841	0.1342	-0.6261	5.3190E-01	7.0920E-01
15-HETE	Oxylipin	0.0928	0.1495	0.6205	5.3561E-01	7.1094E-01
LPA (18:0)	Lysophospholipid	0.0783	0.1277	0.6134	5.4032E-01	7.1399E-01
w3FA/w6FA	Fatty acid	0.0491	0.0839	0.5849	5.5926E-01	7.3573E-01
LPA (16:0)	Lysophospholipid	0.0696	0.1199	0.5804	5.6225E-01	7.3639E-01
7-HDoHE	Oxylipin	-0.0665	0.1167	-0.5695	5.6962E-01	7.4277E-01
3-AIBA	Amine	0.0531	0.0944	0.5623	5.7456E-01	7.4432E-01
Sum iPs	Oxylipin	0.0728	0.1299	0.5603	5.7584E-01	7.4432E-01
9-HODE	Oxylipin	0.0725	0.1358	0.5337	5.9413E-01	7.6462E-01
LPA (22:4)	Lysophospholipid	-0.0810	0.1536	-0.5276	5.9836E-01	7.6673E-01
19,20-EpDPE	Oxylipin	-0.0760	0.1462	-0.5197	6.0383E-01	7.7040E-01
17,18-DiHETE	Oxylipin	-0.0684	0.1358	-0.5033	6.1527E-01	7.7900E-01
2,3-dinor-8-iso-PGF2alpha	Oxylipin	-0.0775	0.1543	-0.5025	6.1583E-01	7.7900E-01
FA (18:0)	Fatty acid	-0.0710	0.1433	-0.4957	6.2067E-01	7.7919E-01
SIP (18:0)	Lysophospholipid	-0.0683	0.1389	-0.4918	6.2335E-01	7.7919E-01
14,15-DiHETE	Oxylipin	0.0607	0.1240	0.4894	6.2511E-01	7.7919E-01
LPI (16:1)	Lysophospholipid	0.0674	0.1383	0.4874	6.2651E-01	7.7919E-01
LPI (14:0)	Lysophospholipid	0.0557	0.1183	0.4713	6.3792E-01	7.8882E-01
12,13-DiHOME	Oxylipin	-0.0457	0.0974	-0.4689	6.3958E-01	7.8882E-01
Homocitrulline	Amine	-0.0542	0.1238	-0.4378	6.6196E-01	8.1303E-01

Chapter III

Sum HETrEs	Oxylipin	0.0617	0.1449	0.4260	6.7058E-01	8.2022E-01
TXB3	Oxylipin	0.0550	0.1306	0.4215	6.7381E-01	8.2077E-01
Sum HODEs	Oxylipin	0.0569	0.1374	0.4137	6.7953E-01	8.2435E-01
3-Methoxy-tyramine	Amine	0.0644	0.1613	0.3992	6.9017E-01	8.3384E-01
LPA (18:1)	Lysophospholipid	0.0522	0.1332	0.3919	6.9551E-01	8.3687E-01
2-aminoadipic acid	Amine	-0.0435	0.1236	-0.3520	7.2520E-01	8.6907E-01
5-OH-Trp	Amine	0.0495	0.1450	0.3414	7.3320E-01	8.7510E-01
Sum PBA	Bile Acid	0.0497	0.1493	0.3328	7.3960E-01	8.7578E-01
LPA (20:4)	Lysophospholipid	-0.0420	0.1269	-0.3307	7.4121E-01	8.7578E-01
LPE (18:3)	Lysophospholipid	-0.0396	0.1203	-0.3288	7.4263E-01	8.7578E-01
Sum BA	Bile Acid	-0.0498	0.1565	-0.3180	7.5077E-01	8.8185E-01
2,3-dinor-8-iso-PGF2alpha/AA	Oxylipin	-0.0472	0.1511	-0.3122	7.5522E-01	8.8357E-01
20-HETE/AA	Oxylipin	0.0409	0.1372	0.2982	7.6594E-01	8.9238E-01
LPG (18:3)	Lysophospholipid	0.0314	0.1068	0.2944	7.6877E-01	8.9238E-01
delta-17,6-keto-PGF1alpha/EPA	Oxylipin	0.0360	0.1273	0.2829	7.7752E-01	8.9901E-01
Glu	Amine	0.0397	0.1446	0.2743	7.8414E-01	9.0314E-01
Coriolic acid	Oxylipin	0.0346	0.1397	0.2476	8.0468E-01	9.2320E-01
cLPA (18:0)	Lysophospholipid	0.0302	0.1322	0.2287	8.1929E-01	9.3023E-01
LPS (20:4)	Lysophospholipid	0.0256	0.1139	0.2249	8.2233E-01	9.3023E-01
LPG (16:0)	Lysophospholipid	-0.0319	0.1425	-0.2240	8.2297E-01	9.3023E-01
Glutathione	Amine	0.0298	0.1332	0.2234	8.2345E-01	9.3023E-01
Cys/Cystathionine	Amine	-0.0314	0.1432	-0.2194	8.2652E-01	9.3023E-01
Sum PGs	Oxylipin	-0.0322	0.1507	-0.2135	8.3113E-01	9.3187E-01
LPA (18:2)	Lysophospholipid	0.0234	0.1187	0.1973	8.4381E-01	9.4251E-01
Sum HETEs	Oxylipin	0.0289	0.1531	0.1886	8.5059E-01	9.4652E-01
PAF 18(2)	PAF	0.0219	0.1217	0.1803	8.5706E-01	9.4895E-01
TXB3/EPA	Oxylipin	-0.0223	0.1256	-0.1776	8.5919E-01	9.4895E-01
LPG (22:4)	Lysophospholipid	0.0248	0.1428	0.1734	8.6248E-01	9.4905E-01
LPA (22:6)	Lysophospholipid	-0.0217	0.1331	-0.1633	8.7041E-01	9.5422E-01
16-HDoHE/DHA	Oxylipin	0.0231	0.1489	0.1553	8.7671E-01	9.5432E-01
LPA (16:1)	Lysophospholipid	0.0199	0.1281	0.1550	8.7695E-01	9.5432E-01
LPI (20:4)	Lysophospholipid	-0.0187	0.1306	-0.1430	8.8641E-01	9.6109E-01
9-HOTrE	Oxylipin	0.0171	0.1284	0.1332	8.9419E-01	9.6599E-01
5-HEPE	Oxylipin	0.0151	0.1343	0.1121	9.1081E-01	9.7599E-01
ETE	Fatty acid	-0.0156	0.1502	-0.1036	9.1761E-01	9.7599E-01
15-HEPE/EPA	Oxylipin	0.0126	0.1277	0.0987	9.2148E-01	9.7599E-01
13,14-dihydro-15-keto-PGF2alpha/AA	Oxylipin	-0.0138	0.1427	-0.0969	9.2288E-01	9.7599E-01
5-KETE	Oxylipin	0.0147	0.1526	0.0960	9.2362E-01	9.7599E-01
19,20-DiHDPA	Oxylipin	0.0128	0.1418	0.0903	9.2815E-01	9.7599E-01
8-HDoHE/DHA	Oxylipin	0.0130	0.1473	0.0881	9.2988E-01	9.7599E-01
5-aminolevulinic acid	Amine	-0.0117	0.1360	-0.0858	9.3173E-01	9.7599E-01
DHA	Fatty acid	-0.0095	0.1136	-0.0840	9.3313E-01	9.7599E-01
LPI (22:6)	Lysophospholipid	0.0112	0.1409	0.0796	9.3662E-01	9.7619E-01
Sum DiHETEs	Oxylipin	-0.0101	0.1375	-0.0735	9.4148E-01	9.7782E-01
LPE (14:0)	Lysophospholipid	0.0080	0.1331	0.0602	9.5209E-01	9.8538E-01
20-HETE	Oxylipin	0.0078	0.1420	0.0550	9.5620E-01	9.8618E-01
HCA	Bile Acid	-0.0061	0.1334	-0.0459	9.6342E-01	9.8682E-01
LPA (20:3)	Lysophospholipid	-0.0054	0.1182	-0.0458	9.6348E-01	9.8682E-01
16-HDoHE	Oxylipin	0.0041	0.1141	0.0360	9.7131E-01	9.9141E-01
AA	Fatty acid	-0.0043	0.1503	-0.0288	9.7705E-01	9.9384E-01
Cystathionine/HomoCys	Amine	-0.0011	0.1343	-0.0085	9.9321E-01	9.9907E-01
Clupanodonic acid	Fatty acid	0.0009	0.1172	0.0081	9.9355E-01	9.9907E-01
13,14-dihydro-15-keto-PGF2alpha	Oxylipin	-0.0009	0.1386	-0.0066	9.9474E-01	9.9907E-01
9-HEPE/EPA	Oxylipin	0.0004	0.1342	0.0030	9.9758E-01	9.9907E-01
8-HDoHE	Oxylipin	-0.0001	0.1159	-0.0012	9.9907E-01	9.9907E-01

Table S3: Linear mixed-effect model results of the "Sepsis" model comparing non-sepsis groups with sepsis

Metabolite	Category	Estimate	Standard Error	z-value	p-value	Adjusted p-value
LPS (18:0)	Lysophospholipid	0.8331	0.1355	6.1507	3.9959E-09	1.1828E-06
Phe/Tyr	Amine	0.5405	0.0914	5.9100	1.3340E-08	1.9743E-06
Thr	Amine	-0.7182	0.1231	-5.8335	2.0075E-08	1.9807E-06
4-OH-Pro	Amine	-0.7348	0.1284	-5.7221	3.5035E-08	2.0885E-06
LPI (18:0)	Lysophospholipid	0.7428	0.1297	5.7248	3.5278E-08	2.0885E-06
OH-Lys	Amine	-0.7246	0.1315	-5.5107	1.0202E-07	4.4585E-06
5-HT/Trp	Amine	0.7895	0.1435	5.5016	1.0898E-07	4.4585E-06
4-OH-Pro/Pro	Amine	-0.7100	0.1296	-5.4769	1.2050E-07	4.4585E-06
Trp	Amine	-0.6165	0.1134	-5.4372	1.5405E-07	5.0666E-06
LPI (16:0)	Lysophospholipid	0.7070	0.1394	5.0715	8.5322E-07	2.5255E-05
LPE (16:0)	Lysophospholipid	0.5747	0.1233	4.6625	5.5059E-06	1.3857E-04
Cortisol	Steroid Hormone	0.6346	0.1364	4.6520	5.8352E-06	1.3857E-04
Tyr	Amine	-0.5066	0.1092	-4.6398	6.0860E-06	1.3857E-04
Arg	Amine	-0.6311	0.1406	-4.4874	1.1761E-05	2.4866E-04

Diagnosis of Late-Onset Sepsis

ADMA	Amine	-0.6079	0.1371	-4.4325	1.5049E-05	2.9696E-04
AAA	Amine	-0.5344	0.1226	-4.3573	2.0626E-05	3.8158E-04
SIP (18:2)	Lysophospholipid	-0.4744	0.1157	-4.1013	5.8677E-05	1.0217E-03
3-Methoxy-tyrosine	Amine	-0.5410	0.1329	-4.0694	6.6294E-05	1.0902E-03
LPE (20:4)	Lysophospholipid	-0.5007	0.1255	-3.9889	9.1135E-05	1.4104E-03
5-HT	Amine	0.5797	0.1457	3.9795	9.5295E-05	1.4104E-03
BCAA/Tyr	Amine	0.3738	0.0952	3.9272	1.1603E-04	1.6355E-03
Gln	Amine	-0.5582	0.1434	-3.8927	1.3250E-04	1.7828E-03
g-Glu-Gln	Amine	-0.5714	0.1479	-3.8643	1.4766E-04	1.9003E-03
Gly-Pro	Amine	-0.4773	0.1241	-3.8465	1.5909E-04	1.9621E-03
Sum DiHETrEs	Oxylipin	-0.4915	0.1311	-3.7490	2.2838E-04	2.7011E-03
LPE (22:6)	Lysophospholipid	-0.5289	0.1415	-3.7392	2.3726E-04	2.7011E-03
LPE (18:0)	Lysophospholipid	0.4260	0.1163	3.6645	3.1322E-04	3.4338E-03
Trimethyl-Lys	Amine	-0.4564	0.1295	-3.5236	5.2604E-04	5.5610E-03
LPE (22:4)	Lysophospholipid	-0.4166	0.1191	-3.4984	5.6875E-04	5.8052E-03
cLPA (16:1)	Lysophospholipid	-0.4753	0.1372	-3.4634	6.4400E-04	6.3541E-03
Citrulline	Amine	-0.4165	0.1208	-3.4476	6.8284E-04	6.4389E-03
LPS (22:4)	Lysophospholipid	0.5050	0.1471	3.4339	7.1386E-04	6.4389E-03
Met	Amine	-0.4832	0.1408	-3.4324	7.1785E-04	6.4389E-03
LPE (20:3)	Lysophospholipid	-0.4402	0.1292	-3.4063	7.8592E-04	6.8421E-03
8,9-DiHETrE	Oxylipin	-0.4683	0.1384	-3.3824	8.5402E-04	7.0737E-03
Saccharopine	Amine	-0.5040	0.1491	-3.3793	8.6323E-04	7.0737E-03
Sum OG	Endocannabinoid	-0.4988	0.1479	-3.3728	8.8422E-04	7.0737E-03
Sphinganine 18.0	Lysophospholipid	0.5019	0.1497	3.3529	9.5030E-04	7.4023E-03
5-KETE/5-HETE	Oxylipin	0.4521	0.1360	3.3251	1.0651E-03	8.0838E-03
PGF2alpha/AA	Oxylipin	0.4793	0.1462	3.2774	1.2216E-03	9.0399E-03
11,12-DiHETrE	Oxylipin	-0.4220	0.1302	-3.2403	1.3835E-03	9.9879E-03
Asn	Amine	-0.3473	0.1101	-3.1536	1.8634E-03	1.2946E-02
Gln/Glu	Amine	-0.4871	0.1546	-3.1504	1.8807E-03	1.2946E-02
Homoserine	Amine	-0.4295	0.1394	-3.0798	2.3422E-03	1.5756E-02
Lys	Amine	-0.4175	0.1362	-3.0647	2.4586E-03	1.5998E-02
Arg/Lys	Amine	-0.4540	0.1482	-3.0632	2.4862E-03	1.5998E-02
PGE1	Oxylipin	0.4737	0.1550	3.0559	2.5413E-03	1.6005E-02
His	Amine	-0.4039	0.1336	-3.0234	2.8178E-03	1.6809E-02
DHEA	Endocannabinoid	0.2512	0.0832	3.0177	2.8567E-03	1.6809E-02
LPS (16:0)	Lysophospholipid	0.4430	0.1470	3.0142	2.8893E-03	1.6809E-02
PGF2alpha	Oxylipin	0.4697	0.1559	3.0132	2.8962E-03	1.6809E-02
Sum KETEs	Oxylipin	0.4346	0.1451	2.9955	3.0616E-03	1.7211E-02
PGE2/AA	Oxylipin	0.4439	0.1483	2.9941	3.0816E-03	1.7211E-02
5,6-DiHETrE	Oxylipin	-0.3832	0.1284	-2.9848	3.1667E-03	1.7358E-02
LCA	Bile Acid	-0.4104	0.1384	-2.9662	3.3739E-03	1.8158E-02
S-Methyl-Cys	Amine	-0.4013	0.1358	-2.9558	3.4692E-03	1.8337E-02
BCAA/AAA	Amine	0.3063	0.1046	2.9300	3.7572E-03	1.9511E-02
Putrescine	Amine	0.3933	0.1369	2.8738	4.4667E-03	2.2796E-02
LPI (18:1)	Lysophospholipid	0.3964	0.1387	2.8571	4.7150E-03	2.3655E-02
LPE (18:2)	Lysophospholipid	-0.3600	0.1270	-2.8354	5.0152E-03	2.4742E-02
Sphingosine 18.1	Lysophospholipid	0.4259	0.1513	2.8148	5.3486E-03	2.5648E-02
Ser	Amine	-0.4021	0.1429	-2.8144	5.3723E-03	2.5648E-02
12,13-EpOME/LA	Oxylipin	-0.3630	0.1337	-2.7149	7.1785E-03	3.3728E-02
DEA	Endocannabinoid	0.4026	0.1490	2.7020	7.4792E-03	3.4591E-02
Ornithine	Amine	-0.3620	0.1349	-2.6837	7.8591E-03	3.5481E-02
LPS (22:6)	Lysophospholipid	0.2890	0.1078	2.6800	7.9330E-03	3.5481E-02
OH-Lys/Lys	Amine	-0.3524	0.1317	-2.6764	8.0313E-03	3.5481E-02
1-Met-His	Amine	-0.3679	0.1386	-2.6550	8.5250E-03	3.7109E-02
SDMA	Amine	-0.3246	0.1231	-2.6364	8.9892E-03	3.8562E-02
14,15-DiHETrE	Oxylipin	-0.3417	0.1321	-2.5866	1.0355E-02	4.3789E-02
SIP (18:1)	Lysophospholipid	-0.3109	0.1233	-2.5207	1.2463E-02	5.1960E-02
SIP (16:1)	Lysophospholipid	-0.2592	0.1040	-2.4919	1.3479E-02	5.5415E-02
9-KODE/9-HODE	Oxylipin	-0.3293	0.1335	-2.4671	1.4427E-02	5.8499E-02
Ile	Amine	-0.3844	0.1578	-2.4359	1.5691E-02	6.2762E-02
PGE2	Oxylipin	0.3767	0.1561	2.4132	1.6668E-02	6.5784E-02
PGE1/DGLA	Oxylipin	0.3747	0.1557	2.4072	1.6938E-02	6.5971E-02
5-HEPE/EPA	Oxylipin	-0.2248	0.0939	-2.3940	1.7532E-02	6.7395E-02
5-HETE/AA	Oxylipin	-0.3096	0.1313	-2.3587	1.9247E-02	7.3040E-02
Met-SO2	Amine	-0.2665	0.1141	-2.3364	2.0442E-02	7.6593E-02
LPE (20:5)	Lysophospholipid	-0.3162	0.1362	-2.3218	2.1181E-02	7.8368E-02
GABA	Amine	0.3465	0.1496	2.3167	2.1473E-02	7.8468E-02
18-HEPE	Oxylipin	0.3054	0.1321	2.3119	2.1787E-02	7.8646E-02
12-HEPE	Oxylipin	0.3080	0.1350	2.2817	2.3514E-02	8.3858E-02
OA	Fatty acid	-0.3390	0.1508	-2.2475	2.5645E-02	9.0369E-02
Gly	Amine	-0.2865	0.1312	-2.1830	3.0145E-02	1.0497E-01
5-HETrE/DGLA	Oxylipin	-0.2830	0.1301	-2.1747	3.0777E-02	1.0593E-01
LPI (18:2)	Lysophospholipid	0.2371	0.1117	2.1233	3.4876E-02	1.1866E-01
g-Glu-Ala	Amine	-0.2883	0.1372	-2.1007	3.6839E-02	1.2391E-01

Chapter III

12-KETE	Oxylipin	0.2954	0.1423	2.0754	3.9140E-02	1.3017E-01
Sum HEPeEs	Oxylipin	0.2747	0.1327	2.0696	3.9702E-02	1.3057E-01
LPE (16:1)	Lysophospholipid	-0.2831	0.1376	-2.0566	4.1096E-02	1.3367E-01
EPA	Fatty acid	0.1720	0.0843	2.0418	4.2401E-02	1.3642E-01
BCAA	Amine	-0.3011	0.1502	-2.0052	4.6247E-02	1.4669E-01
LPS (18:2)	Lysophospholipid	0.2629	0.1313	2.0022	4.6585E-02	1.4669E-01
Homocitrulline	Amine	-0.2500	0.1255	-1.9931	4.7518E-02	1.4806E-01
14,15-DiHETE	Oxylipin	0.2495	0.1261	1.9792	4.9096E-02	1.5138E-01
Ala	Amine	-0.2843	0.1452	-1.9574	5.1593E-02	1.5744E-01
11,12-DiHETE/11,12-EpETRE	Oxylipin	-0.2520	0.1292	-1.9497	5.2518E-02	1.5843E-01
5-HETE	Oxylipin	-0.2956	0.1519	-1.9459	5.2989E-02	1.5843E-01
TXB1	Oxylipin	0.2705	0.1402	1.9296	5.4971E-02	1.6272E-01
Mead.Acid	Fatty acid	-0.2723	0.1425	-1.9111	5.7355E-02	1.6809E-01
Ornithine/Arg	Amine	0.2985	0.1568	1.9031	5.8403E-02	1.6948E-01
DPA	Fatty acid	-0.2667	0.1435	-1.8593	6.4355E-02	1.8301E-01
Met-SO	Amine	-0.2719	0.1464	-1.8571	6.4667E-02	1.8301E-01
LA	Fatty acid	0.1959	0.1056	1.8554	6.4921E-02	1.8301E-01
Kyn/Trp	Amine	0.2710	0.1494	1.8134	7.1187E-02	1.9728E-01
cLPA (14:0)	Lysophospholipid	-0.1845	0.1019	-1.8110	7.1548E-02	1.9728E-01
15-HEPE	Oxylipin	0.2170	0.1200	1.8083	7.1982E-02	1.9728E-01
5-HETRE	Oxylipin	-0.2445	0.1359	-1.7987	7.3488E-02	1.9956E-01
Glu/GABA	Amine	-0.2456	0.1372	-1.7899	7.4904E-02	2.0156E-01
Carnosine	Amine	-0.2076	0.1176	-1.7660	7.8845E-02	2.1025E-01
GLA	Fatty acid	-0.2507	0.1425	-1.7596	7.9909E-02	2.1119E-01
Leu	Amine	-0.2724	0.1556	-1.7511	8.1440E-02	2.1333E-01
8,12-iso-iPF2alpha-VI	Oxylipin	-0.2631	0.1517	-1.7348	8.4219E-02	2.1867E-01
Gly-Gly	Amine	0.2209	0.1298	1.7012	9.0588E-02	2.3316E-01
8,12-iso-iPF2alpha-VI/AA	Oxylipin	-0.2427	0.1443	-1.6821	9.4062E-02	2.4002E-01
LPA (20:5)	Lysophospholipid	0.2134	0.1277	1.6712	9.6155E-02	2.4326E-01
TLCA-3S	Bile Acid	-0.2464	0.1498	-1.6451	1.0141E-01	2.5369E-01
12-HETE/AA	Oxylipin	0.2550	0.1553	1.6426	1.0199E-01	2.5369E-01
TXB2	Oxylipin	0.2180	0.1349	1.6165	1.0747E-01	2.6508E-01
15-HETE/AA	Oxylipin	0.2380	0.1485	1.6022	1.1058E-01	2.7051E-01
Sum TXs	Oxylipin	0.2250	0.1413	1.5924	1.1279E-01	2.7365E-01
5-KETE	Oxylipin	0.2474	0.1560	1.5861	1.1424E-01	2.7492E-01
15-HETRE	Oxylipin	0.2385	0.1517	1.5728	1.1726E-01	2.7848E-01
15-HETRE/DGLA	Oxylipin	0.2419	0.1539	1.5713	1.1760E-01	2.7848E-01
Val	Amine	-0.2170	0.1399	-1.5510	1.2242E-01	2.8757E-01
Arg/ADMA	Amine	-0.2362	0.1527	-1.5470	1.2338E-01	2.8757E-01
Kyn	Amine	-0.2212	0.1437	-1.5394	1.2522E-01	2.8956E-01
TXB2/AA	Oxylipin	0.2038	0.1331	1.5309	1.2730E-01	2.9211E-01
11-HETE/AA	Oxylipin	0.2316	0.1521	1.5229	1.2929E-01	2.9392E-01
Asp	Amine	0.2246	0.1481	1.5167	1.3098E-01	2.9392E-01
TUDCA	Bile Acid	0.2191	0.1445	1.5159	1.3107E-01	2.9392E-01
LPS (18:1)	Lysophospholipid	0.2329	0.1554	1.4988	1.3545E-01	2.9873E-01
beta-Ala	Amine	-0.2001	0.1336	-1.4976	1.3573E-01	2.9873E-01
Sum BA	Bile Acid	0.2377	0.1589	1.4955	1.3624E-01	2.9873E-01
13-HDoHE/DHA	Oxylipin	0.2242	0.1519	1.4757	1.4150E-01	3.0797E-01
cLPA (20:4)	Lysophospholipid	-0.1966	0.1355	-1.4505	1.4839E-01	3.2062E-01
12-HHTRE	Oxylipin	0.1846	0.1282	1.4397	1.5144E-01	3.2483E-01
11,12-EpETRE/AA	Oxylipin	-0.2018	0.1410	-1.4313	1.5383E-01	3.2757E-01
16-HDoHE/DHA	Oxylipin	0.2150	0.1516	1.4184	1.5753E-01	3.3223E-01
20-HDoHE/DHA	Oxylipin	0.2022	0.1433	1.4111	1.5967E-01	3.3223E-01
11,12-EpETRE	Oxylipin	-0.1776	0.1261	-1.4079	1.6059E-01	3.3223E-01
Cystathionine	Amine	-0.1597	0.1137	-1.4048	1.6160E-01	3.3223E-01
TXB1/DGLA	Oxylipin	0.1994	0.1420	1.4034	1.6195E-01	3.3223E-01
12-HETE	Oxylipin	0.2209	0.1577	1.4009	1.6275E-01	3.3223E-01
9-HEPE	Oxylipin	0.1588	0.1145	1.3869	1.6696E-01	3.3850E-01
LPG (20:4)	Lysophospholipid	-0.1727	0.1254	-1.3774	1.6982E-01	3.4196E-01
12,13-EpOME	Oxylipin	-0.1952	0.1422	-1.3725	1.7135E-01	3.4270E-01
Sarcosine	Amine	-0.1915	0.1408	-1.3602	1.7519E-01	3.4803E-01
LPG (22:6)	Lysophospholipid	0.1290	0.0956	1.3494	1.7866E-01	3.5256E-01
12-HHTRE/AA	Oxylipin	0.1689	0.1258	1.3431	1.8071E-01	3.5423E-01
w3FA/w6FA	Fatty acid	0.1131	0.0855	1.3228	1.8732E-01	3.6478E-01
12,13-DiHODE/12,13-EpOME	Oxylipin	0.1266	0.0960	1.3190	1.8860E-01	3.6487E-01
14-HDoHE/DHA	Oxylipin	0.1948	0.1483	1.3134	1.9054E-01	3.6624E-01
FA (16:0)	Fatty acid	-0.1990	0.1530	-1.3006	1.9484E-01	3.7208E-01
9-HODE/9-HpODE	Oxylipin	0.1844	0.1428	1.2913	1.9805E-01	3.7547E-01
LPE (18:1)	Lysophospholipid	-0.1613	0.1253	-1.2880	1.9915E-01	3.7547E-01
20-HDoHE	Oxylipin	0.1740	0.1360	1.2796	2.0206E-01	3.7642E-01
AEA	Endocannabinoid	0.1420	0.1114	1.2750	2.0382E-01	3.7642E-01
11-HDoHE/DHA	Oxylipin	0.1955	0.1535	1.2736	2.0422E-01	3.7642E-01
11-HETE	Oxylipin	0.1890	0.1486	1.2720	2.0474E-01	3.7642E-01
12-HEPE/EPA	Oxylipin	0.1864	0.1479	1.2610	2.0873E-01	3.8138E-01

Diagnosis of Late-Onset Sepsis

LPA (22:4)	Lysophospholipid	-0.1957	0.1567	-1.2492	2.1298E-01	3.8676E-01
12-KETE/12-HETE	Oxylipin	0.1886	0.1516	1.2441	2.1482E-01	3.8772E-01
O-Acetyl-Ser	Amine	-0.1648	0.1333	-1.2357	2.1796E-01	3.8874E-01
13-HDoHE	Oxylipin	0.1501	0.1215	1.2355	2.1801E-01	3.8874E-01
9-HODE	Oxylipin	0.1700	0.1385	1.2272	2.2112E-01	3.8978E-01
delta-17,6-keto-PGF1alpha	Oxylipin	0.1778	0.1449	1.2268	2.2127E-01	3.8978E-01
14-HDoHE	Oxylipin	0.1950	0.1594	1.2237	2.2254E-01	3.8978E-01
EA	Amine	0.1505	0.1239	1.2146	2.2584E-01	3.9323E-01
Sum SBA	Bile Acid	-0.1955	0.1632	-1.1984	2.3209E-01	4.0175E-01
8-HETrE	Oxylipin	0.1812	0.1525	1.1882	2.3615E-01	4.0565E-01
cLPA (18:0)	Lysophospholipid	0.1596	0.1346	1.1856	2.3709E-01	4.0565E-01
AdA	Fatty acid	-0.1715	0.1459	-1.1752	2.4122E-01	4.1035E-01
8-iso-PGF3alpha	Oxylipin	-0.1171	0.1004	-1.1669	2.4490E-01	4.1320E-01
LPI (22:4)	Lysophospholipid	-0.1564	0.1344	-1.1641	2.4569E-01	4.1320E-01
Sum DiHETEs	Oxylipin	0.1627	0.1408	1.1555	2.4921E-01	4.1676E-01
15-HETE	Oxylipin	0.1746	0.1524	1.1458	2.5317E-01	4.2099E-01
17-HDoHE/DHA	Oxylipin	0.1757	0.1540	1.1409	2.5521E-01	4.2184E-01
Sum PBA	Bile Acid	0.1729	0.1520	1.1377	2.5653E-01	4.2184E-01
8-HETrE/DGLA	Oxylipin	0.1691	0.1496	1.1304	2.5960E-01	4.2453E-01
LPE (14:0)	Lysophospholipid	0.1521	0.1356	1.1215	2.6332E-01	4.2826E-01
16-HDoHE	Oxylipin	0.1301	0.1163	1.1180	2.6482E-01	4.2835E-01
LPI (16:1)	Lysophospholipid	0.1545	0.1411	1.0952	2.7467E-01	4.3963E-01
LPG (18:1)	Lysophospholipid	-0.1644	0.1504	-1.0935	2.7540E-01	4.3963E-01
GCA	Bile Acid	-0.1630	0.1497	-1.0891	2.7737E-01	4.3963E-01
11-HDoHE	Oxylipin	0.1542	0.1417	1.0883	2.7774E-01	4.3963E-01
PAF 18(2)	PAF	0.1331	0.1237	1.0758	2.8322E-01	4.4582E-01
PGF1alpha	Oxylipin	-0.1166	0.1087	-1.0726	2.8466E-01	4.4582E-01
HomoCys	Amine	-0.1516	0.1423	-1.0657	2.8777E-01	4.4831E-01
LPA (20:4)	Lysophospholipid	-0.1370	0.1297	-1.0568	2.9183E-01	4.5019E-01
3-Methoxy-tyramine	Amine	0.1754	0.1660	1.0566	2.9201E-01	4.5019E-01
Glu	Amine	0.1519	0.1488	1.0211	3.0856E-01	4.7324E-01
Sum LG	Endocannabinoid	-0.1256	0.1241	-1.0126	3.1243E-01	4.7669E-01
LPI (14:0)	Lysophospholipid	0.1185	0.1202	0.9854	3.2555E-01	4.9203E-01
Sum HDoHEs	Oxylipin	0.1484	0.1507	0.9850	3.2580E-01	4.9203E-01
LPG (16:0)	Lysophospholipid	0.1394	0.1453	0.9593	3.3851E-01	5.0820E-01
8-HDoHE/DHA	Oxylipin	0.1435	0.1501	0.9564	3.3995E-01	5.0820E-01
17-HDoHE	Oxylipin	0.1247	0.1330	0.9371	3.4975E-01	5.2023E-01
Sum HODEs	Oxylipin	0.1271	0.1404	0.9053	3.6631E-01	5.4213E-01
17,18-DiHETE	Oxylipin	0.1223	0.1381	0.8851	3.7710E-01	5.5533E-01
LPA (22:6)	Lysophospholipid	-0.1195	0.1361	-0.8782	3.8082E-01	5.5584E-01
PAF 16(0)	PAF	-0.1348	0.1540	-0.8750	3.8253E-01	5.5584E-01
18-HEPE/EPA	Oxylipin	0.1218	0.1393	0.8741	3.8308E-01	5.5584E-01
2,3-dinor-8-iso-PGF2alpha/AA	Oxylipin	0.1305	0.1538	0.8485	3.9711E-01	5.7338E-01
19,20-EpDPE	Oxylipin	0.1256	0.1491	0.8423	4.0058E-01	5.7482E-01
LPG (16:1)	Lysophospholipid	-0.1259	0.1500	-0.8394	4.0217E-01	5.7482E-01
LPS (20:4)	Lysophospholipid	-0.0972	0.1166	-0.8337	4.0543E-01	5.7482E-01
8-iso-PGF3alpha/DGLA	Oxylipin	-0.0959	0.1151	-0.8330	4.0587E-01	5.7482E-01
LPG (18:0)	Lysophospholipid	0.1083	0.1317	0.8226	4.1166E-01	5.8024E-01
9-HpODE/LA	Oxylipin	-0.1159	0.1423	-0.8144	4.1633E-01	5.8405E-01
Anserine	Amine	-0.1193	0.1473	-0.8096	4.1910E-01	5.8515E-01
Sum PGs	Oxylipin	0.1221	0.1539	0.7930	4.2865E-01	5.9518E-01
cLPA (18:2)	Lysophospholipid	-0.1016	0.1294	-0.7851	4.3328E-01	5.9518E-01
TXB3	Oxylipin	0.1045	0.1333	0.7835	4.3420E-01	5.9518E-01
HCA	Bile Acid	0.1058	0.1353	0.7821	4.3507E-01	5.9518E-01
Sum AG	Endocannabinoid	-0.1088	0.1397	-0.7792	4.3675E-01	5.9518E-01
AABA	Amine	0.1150	0.1481	0.7764	4.3834E-01	5.9518E-01
8-HDoHE	Oxylipin	0.0902	0.1183	0.7620	4.4692E-01	6.0280E-01
5-aminolevulinic acid	Amine	-0.1050	0.1386	-0.7573	4.4968E-01	6.0280E-01
cLPA (18:1)	Lysophospholipid	-0.0980	0.1296	-0.7566	4.5012E-01	6.0280E-01
PGF1alpha/DGLA	Oxylipin	-0.0934	0.1240	-0.7530	4.5226E-01	6.0280E-01
Sum HETrEs	Oxylipin	0.1115	0.1486	0.7500	4.5414E-01	6.0280E-01
Phe	Amine	0.1062	0.1438	0.7380	4.6138E-01	6.0968E-01
LPE (22:5)	Lysophospholipid	-0.1030	0.1404	-0.7334	4.6410E-01	6.1055E-01
19,20-EpDPE/DHA	Oxylipin	0.0993	0.1374	0.7222	4.7095E-01	6.1683E-01
3-Met-His	Amine	0.1075	0.1506	0.7141	4.7594E-01	6.2061E-01
LPA (20:3)	Lysophospholipid	-0.0850	0.1209	-0.7028	4.8299E-01	6.2704E-01
FA (18:0)	Fatty acid	-0.1006	0.1473	-0.6829	4.9545E-01	6.3966E-01
LPA (14:0)	Lysophospholipid	0.0709	0.1044	0.6789	4.9792E-01	6.3966E-01
19,20-DiHDPA	Oxylipin	0.0982	0.1450	0.6769	4.9919E-01	6.3966E-01
5-OH-Trp	Amine	-0.0988	0.1492	-0.6626	5.0834E-01	6.4857E-01
Cys	Amine	-0.0877	0.1339	-0.6552	5.1307E-01	6.4981E-01
2-aminoadipic acid	Amine	-0.0823	0.1258	-0.6542	5.1370E-01	6.4981E-01
THDCA	Bile Acid	0.0674	0.1047	0.6436	5.2055E-01	6.5416E-01
TCA	Bile Acid	-0.0782	0.1218	-0.6420	5.2156E-01	6.5416E-01

Chapter III

LPE (18:3)	Lysophospholipid	-0.0779	0.1226	-0.6354	5.2583E-01	6.5673E-01
ALA	Fatty acid	0.0631	0.1005	0.6273	5.3110E-01	6.6053E-01
LPI (22:6)	Lysophospholipid	0.0895	0.1437	0.6228	5.3410E-01	6.6149E-01
5- <i>i</i> PF2 α /VI/AA	Oxylipin	0.0861	0.1449	0.5941	5.5311E-01	6.8217E-01
Coriolic acid	Oxylipin	0.0835	0.1429	0.5844	5.5957E-01	6.8727E-01
LPG (18:2)	Lysophospholipid	-0.0713	0.1240	-0.5750	5.6588E-01	6.9215E-01
10-HDoHE/DHA	Oxylipin	0.0861	0.1508	0.5711	5.6854E-01	6.9237E-01
10-HDoHE	Oxylipin	0.0821	0.1447	0.5675	5.7097E-01	6.9237E-01
Tau	Amine	0.0757	0.1347	0.5621	5.7461E-01	6.9237E-01
LPG (20:3)	Lysophospholipid	-0.0848	0.1513	-0.5609	5.7542E-01	6.9237E-01
2,3-dinor-8-iso-PGF2 α	Oxylipin	0.0868	0.1572	0.5520	5.8152E-01	6.9689E-01
O-PO3-EA	Amine	0.0852	0.1559	0.5468	5.8514E-01	6.9839E-01
delta-17,6-keto-PGF1 α /EPA	Oxylipin	0.0703	0.1309	0.5373	5.9166E-01	7.0334E-01
Clupanodonic acid	Fatty acid	0.0607	0.1196	0.5073	6.1249E-01	7.2518E-01
5- <i>i</i> PF2 α /VI	Oxylipin	0.0671	0.1424	0.4711	6.3809E-01	7.5249E-01
Glutathione	Amine	0.0625	0.1360	0.4597	6.4618E-01	7.5708E-01
Sum <i>i</i> Ps	Oxylipin	0.0608	0.1325	0.4584	6.4710E-01	7.5708E-01
9-HEPE/EPA	Oxylipin	-0.0613	0.1380	-0.4444	6.5724E-01	7.6591E-01
LPA (22:5)	Lysophospholipid	0.0581	0.1380	0.4211	6.7412E-01	7.8039E-01
20-HETE/AA	Oxylipin	-0.0595	0.1418	-0.4201	6.7493E-01	7.8039E-01
GCDCA	Bile Acid	0.0465	0.1174	0.3964	6.9220E-01	7.9724E-01
7-HDoHE	Oxylipin	0.0439	0.1194	0.3677	7.1345E-01	8.1853E-01
7-HDoHE/DHA	Oxylipin	0.0547	0.1505	0.3633	7.1675E-01	8.1915E-01
13,14-dihydro-15-keto-PGF2 α	Oxylipin	-0.0471	0.1416	-0.3327	7.3966E-01	8.4207E-01
LPA (18:0)	Lysophospholipid	0.0416	0.1311	0.3169	7.5167E-01	8.5247E-01
SIP (18:0)	Lysophospholipid	-0.0427	0.1419	-0.3010	7.6372E-01	8.6283E-01
LPG (22:4)	Lysophospholipid	-0.0434	0.1464	-0.2965	7.6710E-01	8.6336E-01
20-HETE	Oxylipin	-0.0425	0.1460	-0.2912	7.7122E-01	8.6366E-01
LPG (18:3)	Lysophospholipid	0.0315	0.1093	0.2885	7.7321E-01	8.6366E-01
PGA2/AA	Oxylipin	0.0372	0.1371	0.2716	7.8619E-01	8.7486E-01
Cys/Cystathionine	Amine	0.0380	0.1461	0.2602	7.9499E-01	8.8134E-01
ETE	Fatty acid	-0.0390	0.1540	-0.2532	8.0035E-01	8.8397E-01
5-HEPE	Oxylipin	0.0325	0.1373	0.2364	8.1339E-01	8.9503E-01
9-HOT α /ALA	Oxylipin	-0.0293	0.1306	-0.2241	8.2288E-01	9.0212E-01
Citrulline/Ornithine	Amine	-0.0238	0.1186	-0.2007	8.4116E-01	9.1850E-01
LPG (14:0)	Lysophospholipid	-0.0195	0.0991	-0.1970	8.4402E-01	9.1850E-01
TXB3/EPA	Oxylipin	-0.0239	0.1288	-0.1856	8.5294E-01	9.2333E-01
19,20-DiHDPA/19,20-EpDPE	Oxylipin	-0.0256	0.1397	-0.1833	8.5471E-01	9.2333E-01
DGLA	Fatty acid	0.0265	0.1525	0.1738	8.6218E-01	9.2599E-01
9-HOT α E	Oxylipin	0.0222	0.1318	0.1684	8.6642E-01	9.2599E-01
PGA	Oxylipin	0.0232	0.1417	0.1635	8.7028E-01	9.2599E-01
3-AIBA	Amine	0.0153	0.0957	0.1604	8.7274E-01	9.2599E-01
LPA (16:1)	Lysophospholipid	-0.0211	0.1313	-0.1603	8.7281E-01	9.2599E-01
DHA	Fatty acid	0.0172	0.1162	0.1484	8.8220E-01	9.3261E-01
9-KODE	Oxylipin	-0.0198	0.1379	-0.1434	8.8614E-01	9.3344E-01
LPA (18:2)	Lysophospholipid	-0.0156	0.1217	-0.1281	8.9816E-01	9.3831E-01
9-HpODE	Oxylipin	0.0165	0.1287	0.1280	8.9827E-01	9.3831E-01
LPA (18:1)	Lysophospholipid	-0.0171	0.1362	-0.1255	9.0027E-01	9.3831E-01
AA	Fatty acid	-0.0169	0.1541	-0.1095	9.1289E-01	9.4813E-01
11 β -PGF2 α /AA	Oxylipin	0.0110	0.1163	0.0943	9.2498E-01	9.5733E-01
LPI (20:4)	Lysophospholipid	0.0094	0.1334	0.0703	9.4403E-01	9.6949E-01
Sum HETEs	Oxylipin	0.0105	0.1568	0.0670	9.4661E-01	9.6949E-01
13,14-dihydro-15-keto-PGF2 α /AA	Oxylipin	-0.0095	0.1460	-0.0648	9.4837E-01	9.6949E-01
15-HEPE/EPA	Oxylipin	0.0082	0.1308	0.0630	9.4984E-01	9.6949E-01
12,13-DiHOME	Oxylipin	-0.0048	0.0994	-0.0485	9.6137E-01	9.7789E-01
11 β -PGF2 α	Oxylipin	-0.0029	0.0926	-0.0313	9.7511E-01	9.8770E-01
Pro	Amine	-0.0041	0.1480	-0.0280	9.7769E-01	9.8770E-01
LPA (16:0)	Lysophospholipid	-0.0017	0.1228	-0.0141	9.8878E-01	9.9551E-01
CA	Bile Acid	-0.0007	0.1388	-0.0051	9.9596E-01	9.9677E-01
Cystathionine/HomoCys	Amine	-0.0006	0.1369	-0.0041	9.9677E-01	9.9677E-01

Table S4: Linear mixed-effect model results of the "C_SINS" model comparing control with systemic inflammation-no sepsis

Metabolite	Category	Estimate	Standard Error	z-value	p-value	Adjusted p-value
Trp	Amine	-0.5722	0.1291	-4.4329	2.0105E-05	5.9510E-03
LPS (18:0)	Lysophospholipid	0.6675	0.1580	4.2239	4.6607E-05	6.8979E-03
Gln	Amine	-0.7466	0.1819	-4.1046	7.2418E-05	7.1453E-03
Ornithine	Amine	-0.5843	0.1567	-3.7298	2.9195E-04	1.8318E-02
g-Glu-Gln	Amine	-0.7013	0.1886	-3.7182	3.0942E-04	1.8318E-02
PGF1 α	Oxylipin	-0.4515	0.1236	-3.6538	3.7353E-04	1.8427E-02
Thr	Amine	-0.4880	0.1443	-3.3826	9.5501E-04	4.0383E-02
Sum SBA	Bile Acid	-0.6379	0.1954	-3.2648	1.4294E-03	5.2888E-02

Diagnosis of Late-Onset Sepsis

Saccharopine	Amine	-0.6059	0.1903	-3.1842	1.8606E-03	6.1192E-02
Ser	Amine	-0.5783	0.1854	-3.1190	2.2684E-03	6.7145E-02
Sum OG	Endocannabinoid	-0.5284	0.1739	-3.0384	2.9301E-03	7.6017E-02
LCA	Bile Acid	-0.5120	0.1695	-3.0206	3.0818E-03	7.6017E-02
Gly	Amine	-0.5068	0.1725	-2.9378	3.9492E-03	8.9920E-02
Citrulline/Ornithine	Amine	0.3635	0.1261	2.8825	4.6315E-03	9.5248E-02
Sum DiHETErs	Oxylipin	-0.4713	0.1641	-2.8720	4.8268E-03	9.5248E-02
His	Amine	-0.4835	0.1715	-2.8189	5.6806E-03	1.0062E-01
Gln/Glu	Amine	-0.5342	0.1914	-2.7917	6.1041E-03	1.0062E-01
Cortisol	Steroid Hormone	0.4892	0.1761	2.7781	6.2885E-03	1.0062E-01
5-HETE/AA	Oxylipin	-0.4195	0.1514	-2.7710	6.4588E-03	1.0062E-01
4-OH-Pro	Amine	-0.4357	0.1586	-2.7466	6.8759E-03	1.0176E-01
8,9-DiHETE	Oxylipin	-0.4582	0.1720	-2.6634	8.7321E-03	1.2308E-01
OH-Lys	Amine	-0.4650	0.1765	-2.6344	9.4594E-03	1.2500E-01
cLPA (16:1)	Lysophospholipid	-0.4583	0.1752	-2.6163	9.9418E-03	1.2500E-01
cLPA (14:0)	Lysophospholipid	-0.3446	0.1320	-2.6095	1.0135E-02	1.2500E-01
19,20-EpDPE/DHA	Oxylipin	-0.3874	0.1494	-2.5925	1.0624E-02	1.2579E-01
Lys	Amine	-0.4623	0.1855	-2.4927	1.3971E-02	1.5457E-01
SDMA	Amine	-0.4039	0.1623	-2.4885	1.4099E-02	1.5457E-01
5,6-DiHETE	Oxylipin	-0.4073	0.1655	-2.4608	1.5236E-02	1.5842E-01
SIP (18:2)	Lysophospholipid	-0.3375	0.1374	-2.4557	1.5521E-02	1.5842E-01
19,20-EpDPE	Oxylipin	-0.4704	0.1932	-2.4344	1.6309E-02	1.6091E-01
ADMA	Amine	-0.4194	0.1749	-2.3984	1.8015E-02	1.7202E-01
Cys	Amine	-0.4180	0.1778	-2.3502	2.0486E-02	1.8514E-01
TLCA-3S	Bile Acid	-0.4592	0.1958	-2.3455	2.0641E-02	1.8514E-01
5-HETE	Oxylipin	-0.4492	0.1956	-2.2961	2.3464E-02	1.9430E-01
BCAA	Amine	-0.4437	0.1934	-2.2942	2.3484E-02	1.9430E-01
Ile	Amine	-0.4604	0.2010	-2.2911	2.3631E-02	1.9430E-01
Val	Amine	-0.4116	0.1812	-2.2712	2.4882E-02	1.9905E-01
PAF 16(0)	PAF	-0.4450	0.1999	-2.2261	2.7728E-02	2.1598E-01
8-HDoHE/DHA	Oxylipin	-0.4077	0.1861	-2.1910	3.0276E-02	2.2979E-01
9-HpODE/LA	Oxylipin	-0.4218	0.1972	-2.1394	3.4288E-02	2.5199E-01
14-HDoHE/DHA	Oxylipin	0.4314	0.2023	2.1328	3.4904E-02	2.5199E-01
EA	Amine	0.3126	0.1500	2.0832	3.9203E-02	2.6357E-01
17,18-DiHETE	Oxylipin	-0.3631	0.1747	-2.0781	3.9689E-02	2.6357E-01
cLPA (18:2)	Lysophospholipid	-0.3533	0.1704	-2.0732	4.0295E-02	2.6357E-01
Sum BA	Bile Acid	-0.4428	0.2151	-2.0584	4.1639E-02	2.6357E-01
Met	Amine	-0.3791	0.1849	-2.0507	4.2360E-02	2.6357E-01
9-HpODE	Oxylipin	-0.3565	0.1746	-2.0421	4.3230E-02	2.6357E-01
Asn	Amine	-0.2274	0.1115	-2.0394	4.3538E-02	2.6357E-01
S-Methyl-Cys	Amine	-0.3566	0.1760	-2.0261	4.4803E-02	2.6357E-01
LPI (18:0)	Lysophospholipid	0.3133	0.1552	2.0184	4.5811E-02	2.6357E-01
5-HT/Trp	Amine	0.3699	0.1837	2.0131	4.6230E-02	2.6357E-01
11,12-DiHETE	Oxylipin	-0.3319	0.1651	-2.0112	4.6377E-02	2.6357E-01
GCDCA	Bile Acid	-0.3124	0.1563	-1.9984	4.7807E-02	2.6357E-01
16-HDoHE/DHA	Oxylipin	-0.3883	0.1946	-1.9951	4.8120E-02	2.6357E-01
7-HDoHE/DHA	Oxylipin	-0.4042	0.2034	-1.9873	4.8994E-02	2.6357E-01
Sum AG	Endocannabinoid	-0.3434	0.1734	-1.9804	4.9865E-02	2.6357E-01
O-PO3-EA	Amine	0.3811	0.1950	1.9543	5.3021E-02	2.7515E-01
5-KETE	Oxylipin	-0.4304	0.2215	-1.9429	5.4318E-02	2.7515E-01
Tau	Amine	0.3539	0.1833	1.9313	5.5619E-02	2.7515E-01
Sum LG	Endocannabinoid	-0.3149	0.1637	-1.9237	5.6674E-02	2.7515E-01
PGF1alpha/DGLA	Oxylipin	-0.3000	0.1560	-1.9226	5.6865E-02	2.7515E-01
Kyn	Amine	-0.3314	0.1743	-1.9010	5.9615E-02	2.7515E-01
LPE (22:6)	Lysophospholipid	-0.3534	0.1866	-1.8941	6.0592E-02	2.7515E-01
Arg	Amine	-0.3551	0.1879	-1.8894	6.1110E-02	2.7515E-01
PAF 18(2)	PAF	-0.3096	0.1639	-1.8886	6.1218E-02	2.7515E-01
Leu	Amine	-0.3852	0.2039	-1.8889	6.1352E-02	2.7515E-01
Anserine	Amine	-0.2946	0.1611	-1.8287	6.9765E-02	3.0454E-01
LPG (14:0)	Lysophospholipid	-0.2197	0.1202	-1.8272	6.9963E-02	3.0454E-01
LPS (18:1)	Lysophospholipid	0.3686	0.2031	1.8155	7.1839E-02	3.0818E-01
19,20-DiHDP/19,20-EpDPE	Oxylipin	0.3221	0.1800	1.7892	7.5942E-02	3.2113E-01
7-HDoHE	Oxylipin	-0.2890	0.1632	-1.7713	7.8865E-02	3.2590E-01
GCA	Bile Acid	-0.3496	0.1975	-1.7700	7.9272E-02	3.2590E-01
2,3-dinor-8-iso-PGF2alpha	Oxylipin	-0.3805	0.2164	-1.7583	8.1060E-02	3.2868E-01
O-Acetyl-Ser	Amine	-0.2915	0.1686	-1.7294	8.6125E-02	3.4450E-01
LPG (20:3)	Lysophospholipid	-0.3239	0.1889	-1.7151	8.8714E-02	3.4614E-01
LPE (20:3)	Lysophospholipid	-0.2846	0.1660	-1.7143	8.8873E-02	3.4614E-01
11,12-EpETE/AA	Oxylipin	-0.3007	0.1760	-1.7082	9.0085E-02	3.4630E-01
9-HOTE/ALA	Oxylipin	-0.2974	0.1757	-1.6922	9.3327E-02	3.4914E-01
Pro	Amine	-0.3177	0.1882	-1.6884	9.3962E-02	3.4914E-01
TCA	Bile Acid	-0.2405	0.1426	-1.6866	9.4363E-02	3.4914E-01
2,3-dinor-8-iso-PGF2alpha/AA	Oxylipin	-0.3615	0.2155	-1.6773	9.5930E-02	3.5056E-01
14,15-DiHETE	Oxylipin	-0.2885	0.1740	-1.6575	9.9910E-02	3.6065E-01

Chapter III

16-HDoHE	Oxylipin	-0.2564	0.1556	-1.6483	1.0171E-01	3.6272E-01
Sum DiHETEs	Oxylipin	-0.2896	0.1775	-1.6317	1.0545E-01	3.7158E-01
9-KODE	Oxylipin	-0.3017	0.1872	-1.6118	1.0943E-01	3.7734E-01
cLPA (18:1)	Lysophospholipid	-0.2752	0.1716	-1.6037	1.1132E-01	3.7734E-01
14,15-DiHETE	Oxylipin	-0.2579	0.1608	-1.6040	1.1141E-01	3.7734E-01
DEA	Endocannabinoid	0.3206	0.2003	1.6009	1.1218E-01	3.7734E-01
8-HDoHE	Oxylipin	-0.2485	0.1588	-1.5655	1.1990E-01	3.8944E-01
4-OH-Pro/Pro	Amine	-0.2746	0.1755	-1.5647	1.2024E-01	3.8944E-01
PGE1/DGLA	Oxylipin	0.3121	0.2002	1.5587	1.2164E-01	3.8944E-01
HCA	Bile Acid	-0.2880	0.1850	-1.5570	1.2190E-01	3.8944E-01
Ala	Amine	-0.2905	0.1879	-1.5461	1.2453E-01	3.8944E-01
LPE (22:4)	Lysophospholipid	-0.2677	0.1732	-1.5455	1.2473E-01	3.8944E-01
PGA2/AA	Oxylipin	0.2487	0.1613	1.5421	1.2560E-01	3.8944E-01
S1P (18:1)	Lysophospholipid	-0.2237	0.1452	-1.5399	1.2630E-01	3.8944E-01
PGE2/AA	Oxylipin	0.2791	0.1836	1.5202	1.3092E-01	3.9952E-01
cLPA (20:4)	Lysophospholipid	-0.2595	0.1748	-1.4849	1.4019E-01	4.1884E-01
LPE (20:4)	Lysophospholipid	-0.2464	0.1665	-1.4798	1.4150E-01	4.1884E-01
14-HDoHE	Oxylipin	0.3085	0.2088	1.4778	1.4204E-01	4.1884E-01
11,12-EpTrE	Oxylipin	-0.2466	0.1682	-1.4666	1.4497E-01	4.1884E-01
AAA	Amine	-0.2330	0.1593	-1.4633	1.4582E-01	4.1884E-01
LPE (18:2)	Lysophospholipid	-0.2565	0.1759	-1.4589	1.4706E-01	4.1884E-01
LPE (20:5)	Lysophospholipid	-0.2788	0.1912	-1.4584	1.4716E-01	4.1884E-01
11beta-PGF2alpha	Oxylipin	-0.1838	0.1276	-1.4411	1.5300E-01	4.2824E-01
CA	Bile Acid	0.2548	0.1778	1.4332	1.5420E-01	4.2824E-01
LPE (22:5)	Lysophospholipid	-0.2953	0.2063	-1.4316	1.5480E-01	4.2824E-01
11beta-PGF2alpha/AA	Oxylipin	-0.2422	0.1704	-1.4209	1.5804E-01	4.3314E-01
PGF2alpha	Oxylipin	0.2742	0.1971	1.3911	1.6658E-01	4.5237E-01
12-HETE/AA	Oxylipin	0.2924	0.2132	1.3715	1.7273E-01	4.5993E-01
S1P (16:1)	Lysophospholipid	-0.1729	0.1261	-1.3710	1.7291E-01	4.5993E-01
12-HEPE/EPA	Oxylipin	0.2769	0.2031	1.3637	1.7514E-01	4.5993E-01
HomoCys	Amine	-0.2844	0.2088	-1.3623	1.7558E-01	4.5993E-01
TUDCA	Bile Acid	-0.2082	0.1535	-1.3563	1.7750E-01	4.6088E-01
LPG (16:1)	Lysophospholipid	-0.2567	0.1962	-1.3083	1.9320E-01	4.9727E-01
Cystathionine	Amine	-0.2170	0.1669	-1.3008	1.9563E-01	4.9919E-01
9-KODE/9-HODE	Oxylipin	-0.2264	0.1751	-1.2930	1.9846E-01	5.0052E-01
LPG (16:0)	Lysophospholipid	-0.2364	0.1833	-1.2895	1.9953E-01	5.0052E-01
Sum HEPes	Oxylipin	0.2185	0.1745	1.2524	2.1275E-01	5.2463E-01
Met-SO2	Amine	-0.1895	0.1514	-1.2515	2.1299E-01	5.2463E-01
PGE2	Oxylipin	0.2376	0.1905	1.2471	2.1466E-01	5.2463E-01
9-HODE/9-HpODE	Oxylipin	0.2282	0.1836	1.2427	2.1623E-01	5.2463E-01
LPE (16:1)	Lysophospholipid	-0.2253	0.1826	-1.2341	2.1974E-01	5.2509E-01
Gly-Pro	Amine	-0.2061	0.1673	-1.2318	2.2027E-01	5.2509E-01
5-HEPE	Oxylipin	-0.2184	0.1781	-1.2267	2.2223E-01	5.2509E-01
5-HEPE/EPA	Oxylipin	-0.1490	0.1219	-1.2222	2.2398E-01	5.2509E-01
ALA	Fatty acid	0.1704	0.1402	1.2149	2.2664E-01	5.2509E-01
BCAA/AAA	Amine	-0.1612	0.1328	-1.2137	2.2707E-01	5.2509E-01
LPG (18:1)	Lysophospholipid	-0.2293	0.1897	-1.2090	2.2888E-01	5.2517E-01
12,13-EpOME/LA	Oxylipin	-0.2209	0.1845	-1.1975	2.3330E-01	5.3121E-01
9-HODE	Oxylipin	-0.2155	0.1837	-1.1730	2.4300E-01	5.4588E-01
12-HETE	Oxylipin	0.2537	0.2165	1.1720	2.4343E-01	5.4588E-01
8-HETrE/DGLA	Oxylipin	0.2388	0.2054	1.1626	2.4716E-01	5.4757E-01
LPE (16:0)	Lysophospholipid	0.1931	0.1664	1.1608	2.4789E-01	5.4757E-01
Sum PGs	Oxylipin	-0.2173	0.1917	-1.1337	2.5903E-01	5.6210E-01
8-iso-PGF3alpha	Oxylipin	-0.1511	0.1330	-1.1357	2.5905E-01	5.6210E-01
DGLA	Fatty acid	-0.2227	0.1969	-1.1311	2.6016E-01	5.6210E-01
20-HETE/AA	Oxylipin	0.1969	0.1771	1.1116	2.6876E-01	5.7340E-01
12,13-DiHOME	Oxylipin	-0.1553	0.1402	-1.1080	2.6997E-01	5.7340E-01
PGA2	Oxylipin	0.2038	0.1845	1.1046	2.7136E-01	5.7340E-01
18-HEPE/EPA	Oxylipin	0.2088	0.1898	1.1001	2.7362E-01	5.7340E-01
11-HDoHE/DHA	Oxylipin	0.2280	0.2098	1.0869	2.7920E-01	5.7340E-01
12-HEPE	Oxylipin	0.1938	0.1789	1.0832	2.8079E-01	5.7340E-01
15-HETE/AA	Oxylipin	-0.2149	0.1984	-1.0831	2.8085E-01	5.7340E-01
Sum HODEs	Oxylipin	-0.2010	0.1856	-1.0830	2.8089E-01	5.7340E-01
11-HETE/AA	Oxylipin	-0.2207	0.2051	-1.0761	2.8394E-01	5.7566E-01
Tyr	Amine	-0.1560	0.1465	-1.0644	2.8915E-01	5.8029E-01
Ornithine/Arg	Amine	-0.2038	0.1918	-1.0621	2.9014E-01	5.8029E-01
LPG (18:2)	Lysophospholipid	-0.1752	0.1663	-1.0536	2.9405E-01	5.8415E-01
Phe/Tyr	Amine	0.1318	0.1277	1.0323	3.0388E-01	5.9965E-01
LPE (14:0)	Lysophospholipid	-0.1859	0.1848	-1.0059	3.1642E-01	6.1305E-01
PGE1	Oxylipin	0.1925	0.1924	1.0001	3.1923E-01	6.1305E-01
LPS (18:2)	Lysophospholipid	0.1520	0.1522	0.9993	3.1956E-01	6.1305E-01
cLPA (18:0)	Lysophospholipid	-0.1773	0.1788	-0.9916	3.2330E-01	6.1305E-01
FA (16:0)	Fatty acid	-0.1981	0.2002	-0.9893	3.2456E-01	6.1305E-01
LPI (16:0)	Lysophospholipid	0.1715	0.1735	0.9884	3.2484E-01	6.1305E-01

Diagnosis of Late-Onset Sepsis

5-HETrE	Oxylipin	-0.1792	0.1814	-0.9878	3.2516E-01	6.1305E-01
Coriolic acid	Oxylipin	-0.1843	0.1881	-0.9794	3.2933E-01	6.1697E-01
12,13-EpOME	Oxylipin	-0.1835	0.1906	-0.9625	3.3761E-01	6.2139E-01
13-HDoHE	Oxylipin	-0.1583	0.1645	-0.9621	3.3780E-01	6.2139E-01
LPG (20:4)	Lysophospholipid	-0.1593	0.1656	-0.9617	3.3798E-01	6.2139E-01
12-HHTrE/AA	Oxylipin	0.1626	0.1708	0.9520	3.4294E-01	6.2578E-01
12-HHTrE	Oxylipin	0.1700	0.1792	0.9486	3.4460E-01	6.2578E-01
8-iso-PGF3alpha/DGLA	Oxylipin	-0.1558	0.1656	-0.9406	3.4890E-01	6.2633E-01
5-HT	Amine	0.1739	0.1850	0.9398	3.4914E-01	6.2633E-01
beta-Ala	Amine	-0.1713	0.1879	-0.9114	3.6380E-01	6.4870E-01
LPI (18:1)	Lysophospholipid	0.1470	0.1625	0.9048	3.6742E-01	6.5124E-01
3-Methoxy-tyrosine	Amine	-0.1516	0.1703	-0.8904	3.7489E-01	6.6053E-01
LPG (22:6)	Lysophospholipid	-0.1037	0.1170	-0.8863	3.7713E-01	6.6053E-01
TXB2	Oxylipin	0.1637	0.1864	0.8782	3.8145E-01	6.6333E-01
OA	Fatty acid	-0.1585	0.1819	-0.8712	3.8532E-01	6.6333E-01
15-HETrE	Oxylipin	-0.1790	0.2055	-0.8710	3.8545E-01	6.6333E-01
TXB2/AA	Oxylipin	0.1555	0.1801	0.8638	3.8932E-01	6.6611E-01
LPS (20:4)	Lysophospholipid	0.1237	0.1460	0.8478	3.9812E-01	6.7726E-01
Sarcosine	Amine	-0.1597	0.1905	-0.8385	4.0332E-01	6.8149E-01
13-HDoHE/DHA	Oxylipin	-0.1676	0.2007	-0.8351	4.0521E-01	6.8149E-01
GLA	Fatty acid	-0.1477	0.1799	-0.8209	4.1320E-01	6.8812E-01
Sum TXs	Oxylipin	0.1643	0.2004	0.8200	4.1380E-01	6.8812E-01
Glu	Amine	-0.1391	0.1715	-0.8114	4.1898E-01	6.9283E-01
12-KETE	Oxylipin	0.1462	0.1861	0.7858	4.3350E-01	7.1286E-01
5-aminolevulinic acid	Amine	0.1530	0.1997	0.7659	4.4511E-01	7.2792E-01
AdA	Fatty acid	-0.1475	0.1978	-0.7453	4.5744E-01	7.4371E-01
15-HETE	Oxylipin	-0.1536	0.2080	-0.7385	4.6159E-01	7.4371E-01
9-HOTrE	Oxylipin	-0.1301	0.1764	-0.7375	4.6231E-01	7.4371E-01
Sum HDoHEs	Oxylipin	0.1426	0.1976	0.7218	4.7179E-01	7.5274E-01
10-HDoHE/DHA	Oxylipin	0.1485	0.2062	0.7199	4.7301E-01	7.5274E-01
Sum PBA	Bile Acid	-0.1453	0.2063	-0.7040	4.8271E-01	7.6408E-01
Trimethyl-Lys	Amine	-0.1207	0.1738	-0.6943	4.8874E-01	7.6951E-01
Clupanodonic acid	Fatty acid	-0.1112	0.1615	-0.6885	4.9238E-01	7.6982E-01
11-HETE	Oxylipin	-0.1410	0.2074	-0.6795	4.9802E-01	7.6982E-01
PGF2alpha/AA	Oxylipin	0.1288	0.1896	0.6795	4.9804E-01	7.6982E-01
g-Glu-Ala	Amine	-0.1280	0.1900	-0.6740	5.0159E-01	7.6982E-01
LPI (22:6)	Lysophospholipid	-0.1224	0.1820	-0.6727	5.0236E-01	7.6982E-01
LPE (18:1)	Lysophospholipid	-0.1177	0.1758	-0.6693	5.0454E-01	7.6982E-01
Homocitrulline	Amine	0.1075	0.1626	0.6610	5.0980E-01	7.7121E-01
LPE (18:3)	Lysophospholipid	-0.1123	0.1702	-0.6596	5.1067E-01	7.7121E-01
19,20-DiHDPA	Oxylipin	-0.1262	0.1952	-0.6467	5.1908E-01	7.7993E-01
Sum KETEs	Oxylipin	0.1289	0.2033	0.6341	5.2716E-01	7.8807E-01
1-Met-His	Amine	-0.1266	0.2034	-0.6221	5.3502E-01	7.9581E-01
20-HDoHE/DHA	Oxylipin	0.1198	0.1996	0.6001	5.4952E-01	8.1328E-01
w3FA/w6FA	Fatty acid	-0.0658	0.1115	-0.5900	5.5627E-01	8.1402E-01
13,14-dihydro-15-keto-PGF2alpha/AA	Oxylipin	-0.1107	0.1881	-0.5888	5.5703E-01	8.1402E-01
Glu/GABA	Amine	0.0984	0.1680	0.5860	5.5891E-01	8.1402E-01
Homoserine	Amine	-0.1023	0.1755	-0.5829	5.6101E-01	8.1402E-01
11,12-DiHETrE/11,12-EpETrE	Oxylipin	-0.0929	0.1626	-0.5714	5.6871E-01	8.2116E-01
LPI (18:2)	Lysophospholipid	-0.0768	0.1410	-0.5448	5.8689E-01	8.4128E-01
3-Methoxy-tyramine	Amine	-0.1039	0.1914	-0.5428	5.8833E-01	8.4128E-01
DHA	Fatty acid	-0.0798	0.1546	-0.5163	6.0651E-01	8.5915E-01
Kyn/Trp	Amine	0.0904	0.1760	0.5135	6.0849E-01	8.5915E-01
17-HDoHE	Oxylipin	-0.0916	0.1789	-0.5120	6.0953E-01	8.5915E-01
5-OH-Trp	Amine	0.0993	0.1992	0.4985	6.1905E-01	8.6843E-01
18-HEPE	Oxylipin	0.0876	0.1827	0.4798	6.3226E-01	8.7605E-01
Sphinganine 18.0	Lysophospholipid	-0.0959	0.2006	-0.4783	6.3327E-01	8.7605E-01
Cys/Cystathionine	Amine	-0.1002	0.2095	-0.4782	6.3336E-01	8.7605E-01
5-iPF2alpha-VI/AA	Oxylipin	0.0883	0.1896	0.4658	6.4218E-01	8.8275E-01
AABA	Amine	0.0944	0.2063	0.4577	6.4791E-01	8.8275E-01
11-HDoHE	Oxylipin	0.0835	0.1848	0.4518	6.5220E-01	8.8275E-01
15-HEPE	Oxylipin	-0.0679	0.1507	-0.4505	6.5315E-01	8.8275E-01
Carnosine	Amine	-0.0668	0.1485	-0.4500	6.5350E-01	8.8275E-01
TXBI/DGLA	Oxylipin	0.0877	0.1966	0.4464	6.5610E-01	8.8275E-01
Phe	Amine	-0.0820	0.1853	-0.4423	6.5908E-01	8.8275E-01
Sum HETrEs	Oxylipin	-0.0834	0.1944	-0.4290	6.6870E-01	8.9159E-01
3-Met-His	Amine	0.0756	0.1793	0.4216	6.7402E-01	8.9467E-01
8,12-iso-iPF2alpha-VI/AA	Oxylipin	0.0772	0.1948	0.3965	6.9240E-01	9.1281E-01
Arg/ADMA	Amine	-0.0787	0.1994	-0.3945	6.9386E-01	9.1281E-01
LPA (20:3)	Lysophospholipid	0.0628	0.1628	0.3855	7.0052E-01	9.1642E-01
LPA (22:4)	Lysophospholipid	0.0826	0.2160	0.3824	7.0280E-01	9.1642E-01
DHEA	Endocannabinoid	0.0407	0.1092	0.3726	7.1005E-01	9.2182E-01
5-KETE/5-HETE	Oxylipin	0.0688	0.1886	0.3649	7.1587E-01	9.2531E-01
9-HEPE	Oxylipin	-0.0528	0.1493	-0.3538	7.2409E-01	9.2911E-01

Chapter III

3-AIBA	Amine	0.0449	0.1273	0.3525	7.2516E-01	9.2911E-01
LPA (18:2)	Lysophospholipid	-0.0540	0.1551	-0.3483	7.2822E-01	9.2911E-01
8,12-iso-iPF2alpha-VI	Oxylipin	0.0661	0.2018	0.3277	7.4370E-01	9.4367E-01
delta-17,6-keto-PGF1alpha/EPA	Oxylipin	0.0562	0.1749	0.3211	7.4868E-01	9.4367E-01
DPA	Fatty acid	-0.0615	0.1944	-0.3165	7.5217E-01	9.4367E-01
BCAA/Tyr	Amine	-0.0398	0.1258	-0.3162	7.5238E-01	9.4367E-01
13,14-dihydro-15-keto-PGF2alpha	Oxylipin	-0.0561	0.1833	-0.3062	7.5999E-01	9.4682E-01
LA	Fatty acid	0.0445	0.1462	0.3044	7.6130E-01	9.4682E-01
AEA	Endocannabinoid	0.0417	0.1390	0.2998	7.6492E-01	9.4735E-01
Met-SO	Amine	-0.0533	0.1829	-0.2912	7.7133E-01	9.5012E-01
FA (18:0)	Fatty acid	-0.0559	0.1938	-0.2884	7.7357E-01	9.5012E-01
LPA (14:0)	Lysophospholipid	-0.0375	0.1334	-0.2808	7.7932E-01	9.5214E-01
EPA	Fatty acid	-0.0301	0.1103	-0.2732	7.8519E-01	9.5214E-01
15-HEPE/EPA	Oxylipin	-0.0467	0.1718	-0.2715	7.8642E-01	9.5214E-01
17-HDoHE/DHA	Oxylipin	-0.0561	0.2100	-0.2674	7.8961E-01	9.5214E-01
20-HETE	Oxylipin	0.0502	0.1928	0.2604	7.9501E-01	9.5214E-01
TXB3/EPA	Oxylipin	0.0424	0.1670	0.2541	7.9984E-01	9.5214E-01
Mead.AcId	Fatty acid	0.0486	0.1916	0.2535	8.0035E-01	9.5214E-01
Arg/Lys	Amine	-0.0490	0.1938	-0.2526	8.0096E-01	9.5214E-01
ETE	Fatty acid	-0.0503	0.2034	-0.2471	8.0525E-01	9.5341E-01
9-HEPE/EPA	Oxylipin	-0.0443	0.1909	-0.2320	8.1693E-01	9.5890E-01
12-KETE/12-HETE	Oxylipin	-0.0437	0.1979	-0.2209	8.2550E-01	9.5890E-01
LPG (22:4)	Lysophospholipid	0.0410	0.1883	0.2176	8.2810E-01	9.5890E-01
LPS (22:4)	Lysophospholipid	-0.0407	0.1891	-0.2154	8.2982E-01	9.5890E-01
TXB1	Oxylipin	0.0418	0.1970	0.2119	8.3249E-01	9.5890E-01
LPI (22:4)	Lysophospholipid	-0.0378	0.1812	-0.2085	8.3516E-01	9.5890E-01
Gly-Gly	Amine	0.0336	0.1637	0.2050	8.3799E-01	9.5890E-01
LPS (22:6)	Lysophospholipid	0.0260	0.1309	0.1985	8.4294E-01	9.5890E-01
Citrulline	Amine	-0.0292	0.1484	-0.1968	8.4429E-01	9.5890E-01
LPA (20:5)	Lysophospholipid	-0.0335	0.1743	-0.1924	8.4773E-01	9.5890E-01
Sphingosine18.1	Lysophospholipid	-0.0387	0.2093	-0.1848	8.5370E-01	9.5890E-01
LPG (18:3)	Lysophospholipid	-0.0260	0.1408	-0.1846	8.5381E-01	9.5890E-01
5-iPF2alpha-VI	Oxylipin	0.0318	0.1855	0.1714	8.6418E-01	9.5890E-01
OH-Lys/Lys	Amine	-0.0323	0.1908	-0.1693	8.6582E-01	9.5890E-01
LPA (18:1)	Lysophospholipid	-0.0292	0.1762	-0.1656	8.6876E-01	9.5890E-01
Glutathione	Amine	-0.0287	0.1741	-0.1651	8.6915E-01	9.5890E-01
15-HETrE/DGLA	Oxylipin	0.0350	0.2144	0.1633	8.7055E-01	9.5890E-01
LPA (16:1)	Lysophospholipid	-0.0293	0.1862	-0.1572	8.7538E-01	9.5890E-01
Sum iPS	Oxylipin	-0.0281	0.1825	-0.1539	8.7795E-01	9.5890E-01
12,13-DiHOME/12,13-EpOME	Oxylipin	-0.0208	0.1377	-0.1508	8.8040E-01	9.5890E-01
GABA	Amine	-0.0265	0.1823	-0.1452	8.8479E-01	9.5890E-01
10-HDoHE	Oxylipin	0.0275	0.1916	0.1438	8.8588E-01	9.5890E-01
AA	Fatty acid	-0.0295	0.2055	-0.1438	8.8589E-01	9.5890E-01
LPI (14:0)	Lysophospholipid	0.0217	0.1532	0.1416	8.8763E-01	9.5890E-01
TXB3	Oxylipin	-0.0245	0.1838	-0.1331	8.9432E-01	9.6201E-01
LPS (16:0)	Lysophospholipid	-0.0253	0.1988	-0.1273	8.9890E-01	9.6201E-01
20-HDoHE	Oxylipin	0.0235	0.1901	0.1235	9.0194E-01	9.6201E-01
Putrescine	Amine	0.0244	0.2009	0.1215	9.0351E-01	9.6201E-01
LPA (22:6)	Lysophospholipid	0.0215	0.1869	0.1152	9.0846E-01	9.6381E-01
LPI (20:4)	Lysophospholipid	-0.0198	0.1799	-0.1102	9.1240E-01	9.6453E-01
LPI (16:1)	Lysophospholipid	-0.0186	0.1789	-0.1039	9.1739E-01	9.6542E-01
Asp	Amine	-0.0198	0.1963	-0.1010	9.1975E-01	9.6542E-01
LPE (18:0)	Lysophospholipid	0.0158	0.1637	0.0966	9.2321E-01	9.6561E-01
8-HETrE	Oxylipin	-0.0180	0.2052	-0.0879	9.3014E-01	9.6944E-01
5-HETrE/DGLA	Oxylipin	0.0137	0.1667	0.0822	9.3463E-01	9.7070E-01
LPA (22:5)	Lysophospholipid	-0.0135	0.1940	-0.0696	9.4464E-01	9.7550E-01
LPA (16:0)	Lysophospholipid	0.0106	0.1550	0.0681	9.4584E-01	9.7550E-01
THDCA	Bile Acid	-0.0066	0.1284	-0.0511	9.5929E-01	9.8511E-01
LPA (20:4)	Lysophospholipid	0.0080	0.1740	0.0462	9.6323E-01	9.8511E-01
SIP (18:0)	Lysophospholipid	-0.0080	0.1829	-0.0435	9.6534E-01	9.8511E-01
LPG (18:0)	Lysophospholipid	-0.0067	0.1767	-0.0379	9.6985E-01	9.8511E-01
LPA (18:0)	Lysophospholipid	0.0060	0.1693	0.0354	9.7180E-01	9.8511E-01
Cystathionine/HomoCys	Amine	0.0039	0.2025	0.0193	9.8463E-01	9.9415E-01
delta-17,6-keto-PGF1alpha	Oxylipin	-0.0031	0.1936	-0.0158	9.8743E-01	9.9415E-01
Sum HETEs	Oxylipin	0.0016	0.2190	0.0072	9.9429E-01	9.9519E-01
2-aminoadipic acid	Amine	-0.0010	0.1682	-0.0060	9.9519E-01	9.9519E-01

Table S5: Linear mixed-effect model results of the "C_S" model comparing control with sepsis

Metabolite	Category	Estimate	Standard Error	z-value	p-value	Adjusted p-value
Trp	Amine	-0.8421	0.1171	-7.1921	3.4127E-11	1.0102E-08
LPS (18:0)	Lysophospholipid	0.8974	0.1305	6.8784	2.2959E-10	3.3980E-08
Thr	Amine	-0.8666	0.1345	-6.4417	1.5413E-09	1.5189E-07

Diagnosis of Late-Onset Sepsis

Cortisol	Steroid Hormone	0.9284	0.1446	6.4201	2.0526E-09	1.5189E-07
4-OH-Pro	Amine	-0.8327	0.1330	-6.2597	4.0514E-09	2.3984E-07
Phe/Tyr	Amine	0.6143	0.1029	5.9687	1.5184E-08	6.8014E-07
OH-Lys	Amine	-0.8517	0.1429	-5.9620	1.6084E-08	6.8014E-07
LPI (18:0)	Lysophospholipid	0.8345	0.1462	5.7095	5.5238E-08	2.0438E-06
4-OH-Pro/Pro	Amine	-0.8052	0.1426	-5.6478	7.3099E-08	2.4041E-06
ADMA	Amine	-0.8242	0.1498	-5.5010	1.6434E-07	4.8644E-06
Arg	Amine	-0.7911	0.1548	-5.1104	9.1560E-07	2.4638E-05
5-HT/Trp	Amine	0.8342	0.1679	4.9668	1.7823E-06	4.3964E-05
AAA	Amine	-0.6438	0.1304	-4.9382	1.9771E-06	4.5016E-05
Tyr	Amine	-0.5853	0.1192	-4.9094	2.2626E-06	4.7837E-05
Met	Amine	-0.6764	0.1382	-4.8952	2.4988E-06	4.9310E-05
Gln	Amine	-0.7087	0.1489	-4.7583	4.5579E-06	8.4321E-05
SIP (18:2)	Lysophospholipid	-0.5820	0.1262	-4.6115	8.6977E-06	1.4751E-04
LPI (16:0)	Lysophospholipid	0.7316	0.1594	4.5902	8.9704E-06	1.4751E-04
LPE (16:0)	Lysophospholipid	0.5971	0.1353	4.4120	1.8889E-05	2.9427E-04
3-Methoxy-tyrosine	Amine	-0.6226	0.1481	-4.2025	4.3945E-05	6.3563E-04
g-Glu-Gln	Amine	-0.6693	0.1594	-4.1989	4.5095E-05	6.3563E-04
Lys	Amine	-0.5984	0.1437	-4.1636	5.2260E-05	7.0313E-04
Citrulline	Amine	-0.5463	0.1340	-4.0758	7.2990E-05	9.3935E-04
Ornithine	Amine	-0.6028	0.1494	-4.0347	8.8819E-05	1.0954E-03
Sum DiHETrEs	Oxylipin	-0.5646	0.1409	-4.0061	9.5483E-05	1.1305E-03
Ile	Amine	-0.6413	0.1621	-3.9552	1.2120E-04	1.3635E-03
LPE (22:4)	Lysophospholipid	-0.5012	0.1275	-3.9299	1.2747E-04	1.3635E-03
LPE (22:6)	Lysophospholipid	-0.5751	0.1463	-3.9313	1.2898E-04	1.3635E-03
DEA	Endocannabinoid	0.6416	0.1663	3.8574	1.7158E-04	1.7513E-03
LPE (20:4)	Lysophospholipid	-0.5331	0.1391	-3.8314	1.8359E-04	1.8114E-03
S-Methyl-Cys	Amine	-0.5695	0.1491	-3.8197	1.9122E-04	1.8259E-03
8,9-DiHETrE	Oxylipin	-0.5574	0.1488	-3.7470	2.5211E-04	2.3320E-03
His	Amine	-0.5334	0.1433	-3.7230	2.7890E-04	2.5016E-03
Gly-Pro	Amine	-0.5082	0.1379	-3.6861	3.1413E-04	2.6127E-03
Ser	Amine	-0.5543	0.1500	-3.6945	3.1483E-04	2.6127E-03
5-KETE/5-HETE	Oxylipin	0.5794	0.1569	3.6929	3.1776E-04	2.6127E-03
cLPA (16:1)	Lysophospholipid	-0.5193	0.1454	-3.5701	4.7459E-04	3.7967E-03
BCAA/Tyr	Amine	0.3721	0.1055	3.5280	5.4871E-04	4.2742E-03
DHEA	Endocannabinoid	0.3207	0.0916	3.5007	6.0580E-04	4.5590E-03
Sum OG	Endocannabinoid	-0.5741	0.1642	-3.4961	6.1609E-04	4.5590E-03
5,6-DiHETrE	Oxylipin	-0.4883	0.1432	-3.4096	8.3038E-04	5.9949E-03
Asn	Amine	-0.4121	0.1218	-3.3827	9.3996E-04	6.6244E-03
BCAA	Amine	-0.5336	0.1597	-3.3418	1.0572E-03	7.2771E-03
LPE (20:3)	Lysophospholipid	-0.4571	0.1400	-3.2651	1.3460E-03	9.0547E-03
Gln/Glu	Amine	-0.5373	0.1652	-3.2517	1.4586E-03	9.4556E-03
5-HT	Amine	0.5545	0.1714	3.2343	1.4946E-03	9.4556E-03
Gly	Amine	-0.4538	0.1405	-3.2307	1.5106E-03	9.4556E-03
Saccharopine	Amine	-0.5253	0.1629	-3.2252	1.5333E-03	9.4556E-03
9-KODE/9-HODE	Oxylipin	-0.4550	0.1423	-3.1969	1.6942E-03	1.0047E-02
LPE (18:0)	Lysophospholipid	0.4153	0.1300	3.1936	1.6971E-03	1.0047E-02
Leu	Amine	-0.5176	0.1627	-3.1814	1.8036E-03	1.0468E-02
LPS (16:0)	Lysophospholipid	0.5342	0.1697	3.1470	1.9731E-03	1.1231E-02
PGE2/AA	Oxylipin	0.5442	0.1754	3.1018	2.2820E-03	1.2745E-02
PGE1	Oxylipin	0.5455	0.1761	3.0977	2.3362E-03	1.2806E-02
Arg/Lys	Amine	-0.5305	0.1719	-3.0866	2.4128E-03	1.2985E-02
SDMA	Amine	-0.4241	0.1378	-3.0773	2.4605E-03	1.3005E-02
Trimethyl-Lys	Amine	-0.4233	0.1401	-3.0212	2.9736E-03	1.5386E-02
LCA	Bile Acid	-0.4464	0.1479	-3.0182	3.0149E-03	1.5386E-02
11,12-DiHETrE	Oxylipin	-0.4125	0.1396	-2.9550	3.6048E-03	1.8085E-02
5-HETE/AA	Oxylipin	-0.4340	0.1478	-2.9359	3.8870E-03	1.9176E-02
PGF2alpha/AA	Oxylipin	0.4828	0.1700	2.8394	5.1111E-03	2.4802E-02
PGE1/DGLA	Oxylipin	0.4843	0.1745	2.7756	6.1975E-03	2.9588E-02
LPE (18:2)	Lysophospholipid	-0.3896	0.1409	-2.7651	6.3655E-03	2.9811E-02
LPS (22:4)	Lysophospholipid	0.4564	0.1653	2.7612	6.4457E-03	2.9811E-02
1-Met-His	Amine	-0.4137	0.1505	-2.7496	6.6580E-03	3.0319E-02
14,15-DiHETrE	Oxylipin	-0.3914	0.1439	-2.7194	7.2688E-03	3.2599E-02
PGF2alpha	Oxylipin	0.5006	0.1849	2.7080	7.5147E-03	3.3199E-02
SIP (18:1)	Lysophospholipid	-0.3715	0.1374	-2.7035	7.6709E-03	3.3230E-02
cLPA (14:0)	Lysophospholipid	-0.2971	0.1103	-2.6930	7.8417E-03	3.3230E-02
Met-SO2	Amine	-0.3354	0.1244	-2.6964	7.8586E-03	3.3230E-02
Homoserine	Amine	-0.4217	0.1571	-2.6845	8.0334E-03	3.3415E-02
Putrescine	Amine	0.4265	0.1591	2.6804	8.1280E-03	3.3415E-02
Ala	Amine	-0.4044	0.1515	-2.6696	8.4215E-03	3.4147E-02
Val	Amine	-0.4057	0.1529	-2.6526	8.8328E-03	3.5291E-02
LPI (18:1)	Lysophospholipid	0.4359	0.1646	2.6481	8.9420E-03	3.5291E-02
Sum KETEs	Oxylipin	0.4238	0.1623	2.6111	9.8897E-03	3.8518E-02
SIP (16:1)	Lysophospholipid	-0.3084	0.1216	-2.5363	1.2206E-02	4.6923E-02

Chapter III

PGE2	Oxylipin	0.4550	0.1810	2.5136	1.2976E-02	4.9242E-02
LPE (20:5)	Lysophospholipid	-0.3678	0.1491	-2.4663	1.4725E-02	5.5171E-02
18-HEPE	Oxylipin	0.3585	0.1465	2.4473	1.5571E-02	5.7612E-02
12,13-EpOME/LA	Oxylipin	-0.3763	0.1543	-2.4383	1.5862E-02	5.7964E-02
5-HEPE/EPA	Oxylipin	-0.2630	0.1099	-2.3927	1.7906E-02	6.4636E-02
OA	Fatty acid	-0.3987	0.1706	-2.3365	2.0778E-02	7.3911E-02
Sarcosine	Amine	-0.3442	0.1476	-2.3316	2.0975E-02	7.3911E-02
Sphingosine 18.1	Lysophospholipid	0.3924	0.1695	2.3157	2.1940E-02	7.6402E-02
5-HETE	Oxylipin	-0.3934	0.1707	-2.3046	2.2557E-02	7.7637E-02
BCAA/AAA	Amine	0.2569	0.1124	2.2862	2.3564E-02	8.0172E-02
LPS (22:6)	Lysophospholipid	0.2694	0.1225	2.1983	2.9398E-02	9.8883E-02
5-HETrE	Oxylipin	-0.3270	0.1523	-2.1472	3.3352E-02	1.1092E-01
EPA	Fatty acid	0.2012	0.0962	2.0917	3.8055E-02	1.2516E-01
Kyn/Trp	Amine	0.3497	0.1680	2.0817	3.9025E-02	1.2637E-01
Sphinganine 18.0	Lysophospholipid	0.3450	0.1659	2.0796	3.9278E-02	1.2637E-01
LPE (16:1)	Lysophospholipid	-0.3235	0.1582	-2.0450	4.2831E-02	1.3559E-01
g-Glu-Ala	Amine	-0.3062	0.1501	-2.0395	4.3059E-02	1.3559E-01
OH-Lys/Lys	Amine	-0.2982	0.1468	-2.0317	4.3877E-02	1.3671E-01
12-HEPE	Oxylipin	0.3014	0.1513	1.9921	4.8125E-02	1.4838E-01
5-HETrE/DGLA	Oxylipin	-0.2912	0.1474	-1.9754	5.0148E-02	1.5303E-01
Sum HEPEs	Oxylipin	0.2959	0.1536	1.9262	5.5885E-02	1.6879E-01
11,12-EpETrE/AA	Oxylipin	-0.3030	0.1587	-1.9097	5.8065E-02	1.7361E-01
DPA	Fatty acid	-0.2976	0.1570	-1.8952	5.9905E-02	1.7732E-01
Kyn	Amine	-0.2931	0.1581	-1.8543	6.5575E-02	1.9121E-01
FA (16:0)	Fatty acid	-0.3022	0.1631	-1.8528	6.5890E-02	1.9121E-01
cLPA (20:4)	Lysophospholipid	-0.2670	0.1485	-1.7976	7.4168E-02	2.1314E-01
LPI (18:2)	Lysophospholipid	0.2329	0.1300	1.7913	7.5159E-02	2.1391E-01
TXB2	Oxylipin	0.2688	0.1517	1.7723	7.8309E-02	2.2076E-01
LA	Fatty acid	0.2159	0.1225	1.7621	7.9990E-02	2.2145E-01
12-KETE	Oxylipin	0.2817	0.1601	1.7597	8.0383E-02	2.2145E-01
11,12-EpETrE	Oxylipin	-0.2494	0.1419	-1.7573	8.0799E-02	2.2145E-01
TXB1	Oxylipin	0.2768	0.1587	1.7439	8.3109E-02	2.2441E-01
Mead. Acid	Fatty acid	-0.2758	0.1585	-1.7401	8.3887E-02	2.2441E-01
LPA (22:4)	Lysophospholipid	-0.2985	0.1717	-1.7384	8.4155E-02	2.2441E-01
Glu/GABA	Amine	-0.2690	0.1563	-1.7205	8.7355E-02	2.3087E-01
TLCA-3S	Bile Acid	-0.2770	0.1617	-1.7131	8.8643E-02	2.3220E-01
Ornithine/Arg	Amine	0.3079	0.1820	1.6920	9.2669E-02	2.4061E-01
Sum TxS	Oxylipin	0.2660	0.1581	1.6820	9.4551E-02	2.4337E-01
TXB2/AA	Oxylipin	0.2457	0.1479	1.6618	9.8707E-02	2.5187E-01
Arg/ADMA	Amine	-0.2918	0.1765	-1.6535	1.0028E-01	2.5370E-01
LPA (20:4)	Lysophospholipid	-0.2338	0.1434	-1.6303	1.0515E-01	2.6376E-01
LPS (18:2)	Lysophospholipid	0.2376	0.1470	1.6156	1.0831E-01	2.6940E-01
GABA	Amine	0.2695	0.1675	1.6083	1.0987E-01	2.7102E-01
EA	Amine	0.2357	0.1471	1.6025	1.1106E-01	2.7168E-01
LPA (20:5)	Lysophospholipid	0.2341	0.1483	1.5782	1.1650E-01	2.8267E-01
9-HODE/9-HpODE	Oxylipin	0.2527	0.1605	1.5746	1.1749E-01	2.8274E-01
Homocitrulline	Amine	-0.2264	0.1448	-1.5634	1.1995E-01	2.8425E-01
beta-Ala	Amine	-0.2269	0.1452	-1.5630	1.2004E-01	2.8425E-01
20-HDoHE/DHA	Oxylipin	0.2376	0.1577	1.5060	1.3411E-01	3.1148E-01
LPG (22:6)	Lysophospholipid	0.1662	0.1105	1.5044	1.3451E-01	3.1148E-01
TXB1/DGLA	Oxylipin	0.2334	0.1554	1.5021	1.3507E-01	3.1148E-01
14,15-DiHETE	Oxylipin	0.2083	0.1389	1.4997	1.3575E-01	3.1148E-01
O-Acetyl-Ser	Amine	-0.2259	0.1520	-1.4862	1.3927E-01	3.1484E-01
Gly-Gly	Amine	0.2118	0.1425	1.4867	1.3934E-01	3.1484E-01
PAF 18(2)	PAF	0.1954	0.1323	1.4768	1.4171E-01	3.1777E-01
LPE (18:3)	Lysophospholipid	-0.2124	0.1465	-1.4504	1.4893E-01	3.3051E-01
8,12-iso-iPF2alpha-VI	Oxylipin	-0.2432	0.1680	-1.4479	1.4962E-01	3.3051E-01
3-Methoxy-tyramine	Amine	0.2624	0.1824	1.4384	1.5242E-01	3.3210E-01
PGF1alpha	Oxylipin	-0.1749	0.1217	-1.4374	1.5259E-01	3.3210E-01
THDCA	Bile Acid	0.1763	0.1234	1.4282	1.5520E-01	3.3426E-01
Met-SO	Amine	-0.2303	0.1615	-1.4265	1.5584E-01	3.3426E-01
5-KETE	Oxylipin	0.2574	0.1809	1.4223	1.5697E-01	3.3426E-01
TUDCA	Bile Acid	0.2399	0.1693	1.4166	1.5870E-01	3.3535E-01
11-HETE/AA	Oxylipin	0.2506	0.1776	1.4113	1.6013E-01	3.3592E-01
cLPA (18:1)	Lysophospholipid	-0.2059	0.1462	-1.4079	1.6115E-01	3.3592E-01
15-HEPE	Oxylipin	0.1893	0.1351	1.4009	1.6322E-01	3.3667E-01
12-HHTrE	Oxylipin	0.1922	0.1373	1.3995	1.6378E-01	3.3667E-01
12-HETE/AA	Oxylipin	0.2420	0.1755	1.3788	1.7001E-01	3.4705E-01
Sum SBA	Bile Acid	-0.2448	0.1802	-1.3581	1.7649E-01	3.5359E-01
LPE (18:1)	Lysophospholipid	-0.1969	0.1454	-1.3538	1.7773E-01	3.5359E-01
20-HDoHE	Oxylipin	0.1948	0.1439	1.3534	1.7788E-01	3.5359E-01
9-HpODE/LA	Oxylipin	-0.2252	0.1667	-1.3511	1.7859E-01	3.5359E-01
Anserine	Amine	-0.2204	0.1632	-1.3499	1.7918E-01	3.5359E-01
cLPA (18:2)	Lysophospholipid	-0.1886	0.1414	-1.3335	1.8433E-01	3.6134E-01

Diagnosis of Late-Onset Sepsis

11,12-DiHETrE/11,12-EpETrE	Oxylipin	-0.1930	0.1468	-1.3152	1.9036E-01	3.7069E-01
Carnosine	Amine	-0.1750	0.1359	-1.2874	1.9986E-01	3.8629E-01
LPS (18:1)	Lysophospholipid	0.2232	0.1738	1.2844	2.0098E-01	3.8629E-01
15-HETrE/DGLA	Oxylipin	0.2215	0.1732	1.2787	2.0291E-01	3.8750E-01
18-HEPE/EPA	Oxylipin	0.2049	0.1609	1.2734	2.0479E-01	3.8857E-01
14-HDoHE/DHA	Oxylipin	0.2029	0.1599	1.2687	2.0656E-01	3.8944E-01
3-Met-His	Amine	0.2176	0.1739	1.2518	2.1249E-01	3.9808E-01
12,13-EpOME	Oxylipin	-0.1995	0.1600	-1.2472	2.1417E-01	3.9871E-01
LPG (18:1)	Lysophospholipid	-0.2070	0.1682	-1.2312	2.2013E-01	4.0669E-01
8,12-iso-iPF2alpha-VI/AA	Oxylipin	-0.2018	0.1646	-1.2259	2.2216E-01	4.0669E-01
11-HETE	Oxylipin	0.2104	0.1718	1.2245	2.2258E-01	4.0669E-01
12-HHTrE/AA	Oxylipin	0.1602	0.1313	1.2202	2.2457E-01	4.0781E-01
AdA	Fatty acid	-0.1936	0.1593	-1.2150	2.2618E-01	4.0823E-01
LPG (16:1)	Lysophospholipid	-0.2086	0.1762	-1.1839	2.3830E-01	4.2749E-01
15-HETE/AA	Oxylipin	0.1987	0.1719	1.1562	2.4934E-01	4.4435E-01
12-HETE	Oxylipin	0.2053	0.1780	1.1531	2.5070E-01	4.4435E-01
HomoCys	Amine	-0.1841	0.1613	-1.1415	2.5544E-01	4.4648E-01
AEA	Endocannabinoid	0.1452	0.1273	1.1408	2.5584E-01	4.4648E-01
w3FA/w6FA	Fatty acid	0.1143	0.1003	1.1390	2.5643E-01	4.4648E-01
LPI (22:6)	Lysophospholipid	0.1806	0.1600	1.1291	2.6058E-01	4.5037E-01
LPA (22:6)	Lysophospholipid	-0.1756	0.1559	-1.1265	2.6170E-01	4.5037E-01
5-iPF2alpha-VI	Oxylipin	0.1789	0.1609	1.1121	2.6777E-01	4.5814E-01
9-HEPE	Oxylipin	0.1398	0.1280	1.0925	2.7635E-01	4.7003E-01
Cys	Amine	-0.1634	0.1501	-1.0888	2.7789E-01	4.7003E-01
14-HDoHE	Oxylipin	0.1868	0.1726	1.0827	2.8080E-01	4.7225E-01
9-HOTrE/ALA	Oxylipin	-0.1481	0.1374	-1.0783	2.8263E-01	4.7265E-01
LPI (16:1)	Lysophospholipid	0.1738	0.1628	1.0676	2.8737E-01	4.7788E-01
12-kETE/12-HETE	Oxylipin	0.1821	0.1768	1.0300	3.0461E-01	5.0371E-01
13-HDoHE/DHA	Oxylipin	0.1815	0.1772	1.0241	3.0738E-01	5.0404E-01
FA (18:0)	Fatty acid	-0.1581	0.1546	-1.0224	3.0821E-01	5.0404E-01
Cystathionine	Amine	-0.1251	0.1240	-1.0091	3.1448E-01	5.0970E-01
5-iPF2alpha-VI/AA	Oxylipin	0.1765	0.1763	1.0011	3.1843E-01	5.0970E-01
PAF (16:0)	PAF	-0.1673	0.1674	-0.9997	3.1899E-01	5.0970E-01
LPA (20:3)	Lysophospholipid	-0.1337	0.1339	-0.9982	3.1976E-01	5.0970E-01
8-HETrE/DGLA	Oxylipin	0.1652	0.1657	0.9971	3.2029E-01	5.0970E-01
LPG (20:4)	Lysophospholipid	-0.1269	0.1307	-0.9710	3.3311E-01	5.2547E-01
LPG (14:0)	Lysophospholipid	-0.1068	0.1103	-0.9680	3.3458E-01	5.2547E-01
11-HDoHE/DHA	Oxylipin	0.1617	0.1676	0.9646	3.3629E-01	5.2547E-01
12-HEPE/EPA	Oxylipin	0.1588	0.1650	0.9626	3.3729E-01	5.2547E-01
TXB3	Oxylipin	0.1416	0.1523	0.9298	3.5388E-01	5.4842E-01
LPI (22:4)	Lysophospholipid	-0.1418	0.1556	-0.9112	3.6355E-01	5.6037E-01
Sum AG	Endocannabinoid	-0.1442	0.1589	-0.9078	3.6538E-01	5.6037E-01
9-HODE	Oxylipin	0.1395	0.1551	0.8994	3.6986E-01	5.6432E-01
GLA	Fatty acid	-0.1432	0.1602	-0.8942	3.7260E-01	5.6560E-01
LPE (22:5)	Lysophospholipid	-0.1376	0.1553	-0.8863	3.7680E-01	5.6904E-01
LPA (18:1)	Lysophospholipid	-0.1387	0.1607	-0.8633	3.8930E-01	5.8493E-01
Sum DiHETEs	Oxylipin	0.1342	0.1569	0.8557	3.9351E-01	5.8828E-01
ALA	Fatty acid	0.1020	0.1199	0.8505	3.9632E-01	5.8949E-01
O-PO3-EA	Amine	0.1453	0.1727	0.8411	4.0164E-01	5.9442E-01
8-iso-PGF3alpha	Oxylipin	-0.1021	0.1219	-0.8370	4.0419E-01	5.9523E-01
9-HEPE/EPA	Oxylipin	-0.1286	0.1548	-0.8309	4.0742E-01	5.9702E-01
15-HETE	Oxylipin	0.1426	0.1731	0.8234	4.1154E-01	6.0008E-01
13-HDoHE	Oxylipin	0.1095	0.1341	0.8163	4.1560E-01	6.0303E-01
15-HETrE	Oxylipin	0.1395	0.1722	0.8102	4.1908E-01	6.0309E-01
Sum HDoHEs	Oxylipin	0.1312	0.1621	0.8092	4.1971E-01	6.0309E-01
Sum LG	Endocannabinoid	-0.1124	0.1406	-0.7992	4.2536E-01	6.0824E-01
PGF1alpha/DGLA	Oxylipin	-0.1104	0.1402	-0.7876	4.3210E-01	6.1366E-01
LPG (18:2)	Lysophospholipid	-0.1056	0.1344	-0.7856	4.3329E-01	6.1366E-01
19,20-DiHDPA	Oxylipin	0.1173	0.1508	0.7777	4.3791E-01	6.1725E-01
Tau	Amine	0.1129	0.1479	0.7633	4.4643E-01	6.2289E-01
5-OH-Trp	Amine	-0.1251	0.1643	-0.7612	4.4774E-01	6.2289E-01
11-HDoHE	Oxylipin	0.1178	0.1549	0.7604	4.4823E-01	6.2289E-01
GCDA	Bile Acid	0.0985	0.1356	0.7265	4.6867E-01	6.4825E-01
PGA2	Oxylipin	0.1184	0.1640	0.7220	4.7146E-01	6.4867E-01
LPA (16:0)	Lysophospholipid	-0.1029	0.1432	-0.7188	4.7335E-01	6.4867E-01
16-HDoHE/DHA	Oxylipin	0.1197	0.1726	0.6934	4.8908E-01	6.6714E-01
Pro	Amine	-0.0998	0.1448	-0.6892	4.9189E-01	6.6789E-01
17-HDoHE/DHA	Oxylipin	0.1122	0.1705	0.6581	5.1152E-01	6.8416E-01
GCA	Bile Acid	-0.1100	0.1675	-0.6570	5.1213E-01	6.8416E-01
9-KODE	Oxylipin	-0.1025	0.1564	-0.6554	5.1317E-01	6.8416E-01
delta-17,6-keto-PGF1alpha	Oxylipin	0.1034	0.1582	0.6538	5.1430E-01	6.8416E-01
LPS (20:4)	Lysophospholipid	-0.0838	0.1286	-0.6520	5.1543E-01	6.8416E-01
LPA (18:2)	Lysophospholipid	-0.0869	0.1345	-0.6465	5.1896E-01	6.8577E-01
PGA2/AA	Oxylipin	0.1091	0.1701	0.6414	5.2222E-01	6.8701E-01

Chapter III

SIP (18:0)	Lysophospholipid	-0.1011	0.1600	-0.6317	5.2850E-01	6.9220E-01
LPG (18:3)	Lysophospholipid	0.0782	0.1256	0.6227	5.3438E-01	6.9681E-01
LPA (16:1)	Lysophospholipid	-0.0946	0.1538	-0.6152	5.3934E-01	6.9871E-01
12,13-DiHOME/12,13-EpOME	Oxylipin	0.0676	0.1102	0.6133	5.4055E-01	6.9871E-01
LPG (20:3)	Lysophospholipid	-0.0933	0.1545	-0.6042	5.4668E-01	7.0355E-01
8-HETE	Oxylipin	0.1007	0.1688	0.5969	5.5145E-01	7.0662E-01
16-HDoHE	Oxylipin	0.0743	0.1262	0.5886	5.5701E-01	7.1067E-01
Glutathione	Amine	0.0923	0.1588	0.5812	5.6191E-01	7.1360E-01
3-AIBA	Amine	0.0627	0.1089	0.5751	5.6617E-01	7.1360E-01
Sum PBA	Bile Acid	0.1006	0.1752	0.5744	5.6654E-01	7.1360E-01
8-HDoHE/DHA	Oxylipin	0.0978	0.1748	0.5596	5.7657E-01	7.2164E-01
2-aminoacidic acid	Amine	-0.0798	0.1437	-0.5553	5.7946E-01	7.2164E-01
TCA	Bile Acid	-0.0739	0.1341	-0.5508	5.8263E-01	7.2164E-01
5-aminolevulinic acid	Amine	-0.0821	0.1491	-0.5506	5.8267E-01	7.2164E-01
8-iso-PGF3alpha/DGLA	Oxylipin	-0.0744	0.1379	-0.5400	5.9006E-01	7.2765E-01
17-HDoHE	Oxylipin	0.0770	0.1440	0.5343	5.9391E-01	7.2765E-01
Sum HODEs	Oxylipin	0.0837	0.1571	0.5328	5.9491E-01	7.2765E-01
LPA (18:0)	Lysophospholipid	-0.0783	0.1513	-0.5176	6.0555E-01	7.3762E-01
AABA	Amine	0.0779	0.1568	0.4969	6.1995E-01	7.5207E-01
15-HEPE/EPA	Oxylipin	-0.0720	0.1464	-0.4919	6.2349E-01	7.5328E-01
8-HDoHE	Oxylipin	0.0618	0.1292	0.4781	6.3327E-01	7.6199E-01
7-HDoHE/DHA	Oxylipin	-0.0791	0.1683	-0.4703	6.3881E-01	7.6553E-01
9-HPODE	Oxylipin	-0.0680	0.1471	-0.4622	6.4456E-01	7.6646E-01
20-HETE	Oxylipin	-0.0733	0.1587	-0.4620	6.4476E-01	7.6646E-01
Sum BA	Bile Acid	0.0814	0.1785	0.4559	6.4910E-01	7.6853E-01
LPG (22:4)	Lysophospholipid	0.0698	0.1557	0.4482	6.5465E-01	7.7202E-01
17,18-DiHETE	Oxylipin	0.0640	0.1524	0.4203	6.7486E-01	7.9073E-01
Phe	Amine	0.0641	0.1529	0.4189	6.7586E-01	7.9073E-01
12,13-DiHOME	Oxylipin	-0.0471	0.1150	-0.4099	6.8245E-01	7.9336E-01
Sum iPs	Oxylipin	0.0651	0.1596	0.4081	6.8378E-01	7.9336E-01
19,20-DiHDPA/19,20-EpDPE	Oxylipin	0.0610	0.1527	0.3996	6.8997E-01	7.9336E-01
LPI (14:0)	Lysophospholipid	0.0526	0.1321	0.3982	6.9100E-01	7.9336E-01
20-HETE/AA	Oxylipin	-0.0650	0.1639	-0.3969	6.9210E-01	7.9336E-01
LPI (20:4)	Lysophospholipid	0.0599	0.1531	0.3910	6.9631E-01	7.9336E-01
10-HDoHE/DHA	Oxylipin	0.0630	0.1614	0.3903	6.9687E-01	7.9336E-01
DGLA	Fatty acid	-0.0588	0.1669	-0.3524	7.2499E-01	8.2221E-01
11beta-PGF2alpha	Oxylipin	0.0374	0.1127	0.3315	7.4086E-01	8.3701E-01
11beta-PGF2alpha/AA	Oxylipin	0.0445	0.1389	0.3206	7.4903E-01	8.4301E-01
7-HDoHE	Oxylipin	-0.0384	0.1285	-0.2987	7.6559E-01	8.5839E-01
Cys/Cystathionine	Amine	-0.0464	0.1607	-0.2885	7.7331E-01	8.6377E-01
10-HDoHE	Oxylipin	0.0423	0.1538	0.2752	7.8357E-01	8.7194E-01
CA	Bile Acid	0.0422	0.1574	0.2678	7.8924E-01	8.7328E-01
Asp	Amine	0.0423	0.1591	0.2660	7.9068E-01	8.7328E-01
Cystathionine/HomoCys	Amine	0.0403	0.1579	0.2550	7.9907E-01	8.7845E-01
ETE	Fatty acid	-0.0426	0.1691	-0.2521	8.0129E-01	8.7845E-01
Glu	Amine	-0.0372	0.1668	-0.2228	8.2402E-01	9.0004E-01
2,3-dinor-8-iso-PGF2alpha/AA	Oxylipin	0.0380	0.1775	0.2141	8.3073E-01	9.0256E-01
cLPA (18:0)	Lysophospholipid	0.0324	0.1543	0.2099	8.3404E-01	9.0256E-01
2,3-dinor-8-iso-PGF2alpha	Oxylipin	-0.0358	0.1723	-0.2080	8.3548E-01	9.0256E-01
5-HEPE	Oxylipin	0.0311	0.1556	0.2000	8.4178E-01	9.0606E-01
LPG (18:0)	Lysophospholipid	0.0264	0.1474	0.1791	8.5811E-01	9.2029E-01
LPA (14:0)	Lysophospholipid	-0.0205	0.1230	-0.1663	8.6814E-01	9.2769E-01
9-HOTrE	Oxylipin	-0.0221	0.1469	-0.1503	8.8071E-01	9.3530E-01
Coriolic acid	Oxylipin	0.0239	0.1598	0.1492	8.8158E-01	9.3530E-01
AA	Fatty acid	-0.0234	0.1666	-0.1402	8.8870E-01	9.3701E-01
Citrulline/Ornithine	Amine	0.0187	0.1386	0.1348	8.9296E-01	9.3701E-01
LPG (16:0)	Lysophospholipid	0.0225	0.1670	0.1346	8.9313E-01	9.3701E-01
Sum HETEs	Oxylipin	-0.0227	0.1756	-0.1293	8.9733E-01	9.3701E-01
13,14-dihydro-15-keto-PGF2alpha/AA	Oxylipin	-0.0210	0.1650	-0.1271	8.9902E-01	9.3701E-01
19,20-EpDPE	Oxylipin	0.0181	0.1532	0.1184	9.0591E-01	9.4088E-01
delta-17,6-keto-PGF1alpha/EPA	Oxylipin	0.0154	0.1387	0.1111	9.1168E-01	9.4355E-01
Clupanodonic acid	Fatty acid	0.0140	0.1327	0.1055	9.1614E-01	9.4449E-01
HCA	Bile Acid	0.0160	0.1577	0.1018	9.1905E-01	9.4449E-01
13,14-dihydro-15-keto-PGF2alpha	Oxylipin	-0.0158	0.1612	-0.0979	9.2216E-01	9.4449E-01
Sum HETrEs	Oxylipin	0.0145	0.1662	0.0875	9.3038E-01	9.4957E-01
DHA	Fatty acid	0.0106	0.1266	0.0835	9.3353E-01	9.4957E-01
LPA (22:5)	Lysophospholipid	-0.0119	0.1575	-0.0754	9.3998E-01	9.5286E-01
LPE (14:0)	Lysophospholipid	0.0094	0.1513	0.0622	9.5048E-01	9.6021E-01
19,20-EpDPE/DHA	Oxylipin	0.0070	0.1520	0.0462	9.6323E-01	9.6979E-01
Sum PGs	Oxylipin	-0.0039	0.1800	-0.0219	9.8258E-01	9.8591E-01
TXB3/EPA	Oxylipin	-0.0022	0.1529	-0.0143	9.8863E-01	9.8863E-01

Table S6: Linear mixed-effect model results of the "SINS_S" model comparing systemic inflammation-no sepsis with sepsis

Metabolite	Category	Estimate	Standard Error	z-value	p-value	Adjusted p-value
4-OH-Pro/Pro	Amine	-0.7132	0.1853	-3.8493	1.8963E-04	5.6131E-02
Phe/Tyr	Amine	0.3939	0.1087	3.6243	4.3180E-04	6.3907E-02
LPI (16:0)	Lysophospholipid	0.6942	0.2057	3.3755	9.8549E-04	8.3561E-02
5-HT/Trp	Amine	0.6363	0.1919	3.3152	1.2361E-03	8.3561E-02
Putrescine	Amine	0.5058	0.1572	3.2174	1.6671E-03	8.3561E-02
OH-Lys/Lys	Amine	-0.5744	0.1791	-3.2069	1.6938E-03	8.3561E-02
BCAA/Tyr	Amine	0.3694	0.1187	3.1126	2.4411E-03	1.0322E-01
OH-Lys	Amine	-0.5767	0.1903	-3.0296	2.9776E-03	1.0998E-01
4-OH-Pro	Amine	-0.5831	0.1961	-2.9732	3.5451E-03	1.0998E-01
BCAA/AAA	Amine	0.4103	0.1384	2.9644	3.8189E-03	1.0998E-01
Tyr	Amine	-0.3987	0.1357	-2.9388	4.0870E-03	1.0998E-01
LPE (16:0)	Lysophospholipid	0.5092	0.1756	2.8995	4.4790E-03	1.1048E-01
Thr	Amine	-0.5106	0.1806	-2.8268	5.5925E-03	1.2734E-01
LPI (18:0)	Lysophospholipid	0.5102	0.1836	2.7789	6.4725E-03	1.3685E-01
Trp	Amine	-0.4377	0.1631	-2.6842	8.3957E-03	1.4456E-01
Sphinganine 18.0	Lysophospholipid	0.5236	0.1951	2.6838	8.4047E-03	1.4456E-01
LPS (20:4)	Lysophospholipid	-0.3952	0.1471	-2.6855	8.6886E-03	1.4456E-01
LPE (18:0)	Lysophospholipid	0.4023	0.1511	2.6624	8.9408E-03	1.4456E-01
AAA	Amine	-0.4259	0.1603	-2.6564	9.2794E-03	1.4456E-01
3-Methoxy-tyrosine	Amine	-0.5123	0.1977	-2.5907	1.0768E-02	1.5513E-01
2,3-dinor-8-iso-PGF2alpha/AA	Oxylipin	0.4680	0.1809	2.5868	1.1006E-02	1.5513E-01
5-HT	Amine	0.4869	0.1974	2.4667	1.5204E-02	2.0457E-01
Homocitrulline	Amine	-0.4233	0.1733	-2.4423	1.6142E-02	2.0774E-01
1-Met-His	Amine	-0.4127	0.1749	-2.3590	1.9998E-02	2.4665E-01
Gly-Pro	Amine	-0.3926	0.1685	-2.3301	2.1656E-02	2.5640E-01
ADMA	Amine	-0.4507	0.1953	-2.3073	2.2915E-02	2.6087E-01
LPE (20:4)	Lysophospholipid	-0.3747	0.1657	-2.2621	2.5495E-02	2.7719E-01
LPS (16:0)	Lysophospholipid	0.4169	0.1848	2.2565	2.6221E-02	2.7719E-01
Homoserine	Amine	-0.4562	0.2049	-2.2266	2.7817E-02	2.8392E-01
Trimethyl-Lys	Amine	-0.4340	0.1978	-2.1936	3.0060E-02	2.9608E-01
5-HETrE/DGLA	Oxylipin	-0.3787	0.1731	-2.1870	3.1009E-02	2.9608E-01
Arg	Amine	-0.4095	0.1930	-2.1218	3.6136E-02	3.1330E-01
LPS (18:0)	Lysophospholipid	0.4073	0.1919	2.1231	3.6274E-02	3.1330E-01
S1P (18:2)	Lysophospholipid	-0.3501	0.1659	-2.1103	3.6966E-02	3.1330E-01
Sum DiHETrEs	Oxylipin	-0.3735	0.1771	-2.1085	3.7084E-02	3.1330E-01
2,3-dinor-8-iso-PGF2alpha	Oxylipin	0.4128	0.1965	2.1005	3.8104E-02	3.1330E-01
LPE (14:0)	Lysophospholipid	0.3564	0.1734	2.0547	4.2473E-02	3.3433E-01
5-KETE/5-HETE	Oxylipin	0.3466	0.1691	2.0502	4.3308E-02	3.3433E-01
LPS (22:4)	Lysophospholipid	0.4167	0.2045	2.0374	4.4050E-02	3.3433E-01
11,12-DiHETrE	Oxylipin	-0.3466	0.1745	-1.9865	4.9231E-02	3.6431E-01
Sum BA	Bile Acid	0.4268	0.2171	1.9665	5.1562E-02	3.7225E-01
Mead.Acid	Fatty acid	-0.3586	0.1860	-1.9284	5.6305E-02	3.9682E-01
12,13-EpOME/LA	Oxylipin	-0.3435	0.1832	-1.8751	6.3269E-02	4.3553E-01
Sphingosine 18.1	Lysophospholipid	0.3529	0.1907	1.8506	6.7077E-02	4.5125E-01
LPA (20:4)	Lysophospholipid	-0.3142	0.1720	-1.8268	7.0319E-02	4.6254E-01
Arg/Lys	Amine	-0.3373	0.1885	-1.7893	7.6968E-02	4.9527E-01
14,15-DiHETE	Oxylipin	0.2963	0.1705	1.7379	8.5160E-02	5.3633E-01
GABA	Amine	0.3534	0.2087	1.6933	9.3074E-02	5.6953E-01
LPI (18:2)	Lysophospholipid	0.2589	0.1543	1.6772	9.6400E-02	5.6953E-01
14,15-DiHETrE	Oxylipin	-0.3037	0.1830	-1.6597	9.9617E-02	5.6953E-01
Saccharopine	Amine	-0.3328	0.2020	-1.6472	1.0201E-01	5.6953E-01
cLPA (16:1)	Lysophospholipid	-0.3302	0.2014	-1.6395	1.0361E-01	5.6953E-01
LA	Fatty acid	0.2243	0.1370	1.6366	1.0457E-01	5.6953E-01
Sum KETEs	Oxylipin	0.3328	0.2039	1.6320	1.0540E-01	5.6953E-01
Glu/GABA	Amine	-0.3181	0.1951	-1.6302	1.0582E-01	5.6953E-01
LPA (20:3)	Lysophospholipid	-0.2615	0.1618	-1.6160	1.0883E-01	5.7526E-01
Asn	Amine	-0.2794	0.1761	-1.5865	1.1573E-01	6.0052E-01
DHEA	Endocannabinoid	0.1841	0.1167	1.5774	1.1767E-01	6.0052E-01
11,12-DiHETrE/11,12-EpETrE	Oxylipin	-0.2838	0.1813	-1.5652	1.2025E-01	6.0328E-01
LPE (22:6)	Lysophospholipid	-0.2963	0.1916	-1.5468	1.2492E-01	6.1070E-01
LPA (22:6)	Lysophospholipid	-0.2637	0.1717	-1.5357	1.2770E-01	6.1070E-01
OA	Fatty acid	-0.3297	0.2148	-1.5349	1.2792E-01	6.1070E-01
LPI (18:1)	Lysophospholipid	0.2991	0.2005	1.4914	1.3881E-01	6.5221E-01
Met-SO	Amine	-0.2871	0.2024	-1.4182	1.5879E-01	6.8340E-01
5-HETrE	Oxylipin	-0.2473	0.1746	-1.4163	1.5975E-01	6.8340E-01
LPE (16:1)	Lysophospholipid	-0.2527	0.1789	-1.4120	1.6101E-01	6.8340E-01
LPE (20:3)	Lysophospholipid	-0.2553	0.1818	-1.4043	1.6295E-01	6.8340E-01
8,12-iso-iPF2alpha-VI	Oxylipin	-0.2767	0.1975	-1.4009	1.6380E-01	6.8340E-01
LPA (22:4)	Lysophospholipid	-0.2859	0.2047	-1.3969	1.6514E-01	6.8340E-01

Chapter III

delta-17,6-keto-PGF1alpha	Oxylipin	0.2607	0.1873	1.3920	1.6695E-01	6.8340E-01
g-Glu-Ala	Amine	-0.2647	0.1915	-1.3825	1.6938E-01	6.8340E-01
8,9-DiHETE	Oxylipin	-0.2653	0.1927	-1.3768	1.7108E-01	6.8340E-01
LPE (22:5)	Lysophospholipid	0.2390	0.1735	1.3779	1.7112E-01	6.8340E-01
Cortisol	Steroid Hormone	0.2344	0.1705	1.3748	1.7202E-01	6.8340E-01
DEA	Endocannabinoid	0.2434	0.1774	1.3724	1.7316E-01	6.8340E-01
12,13-DiHOME/12,13-EpOME	Oxylipin	0.1646	0.1211	1.3591	1.7655E-01	6.8763E-01
Met	Amine	-0.2682	0.1996	-1.3438	1.8160E-01	6.9666E-01
Met-SO2	Amine	-0.2248	0.1688	-1.3321	1.8518E-01	6.9666E-01
5,6-DiHETE	Oxylipin	-0.2299	0.1728	-1.3306	1.8593E-01	6.9666E-01
17,18-DiHETE	Oxylipin	0.2607	0.1989	1.3108	1.9247E-01	7.1213E-01
5-HEPE/EPA	Oxylipin	-0.1632	0.1255	-1.2999	1.9639E-01	7.1769E-01
Citrulline	Amine	-0.2209	0.1716	-1.2872	2.0050E-01	7.1790E-01
Sum OG	Endocannabinoid	-0.2616	0.2035	-1.2859	2.0130E-01	7.1790E-01
S1P (18:1)	Lysophospholipid	-0.2224	0.1763	-1.2611	2.0974E-01	7.3869E-01
5-OH-Trp	Amine	-0.2521	0.2008	-1.2556	2.1212E-01	7.3869E-01
LPE (18:2)	Lysophospholipid	-0.2175	0.1763	-1.2337	2.1971E-01	7.4996E-01
LPG (14:0)	Lysophospholipid	0.1751	0.1422	1.2315	2.2043E-01	7.4996E-01
LPG (16:0)	Lysophospholipid	0.2562	0.2110	1.2139	2.2723E-01	7.5509E-01
DPA	Fatty acid	-0.2287	0.1891	-1.2091	2.2924E-01	7.5509E-01
CA	Bile Acid	-0.2332	0.1939	-1.2028	2.3137E-01	7.5509E-01
Sum DiHETEs	Oxylipin	0.2216	0.1851	1.1970	2.3423E-01	7.5509E-01
LPI (14:0)	Lysophospholipid	0.2074	0.1741	1.1910	2.3585E-01	7.5509E-01
S-Methyl-Cys	Amine	-0.2313	0.1948	-1.1875	2.3724E-01	7.5509E-01
PGF2alpha/AA	Oxylipin	0.2296	0.1958	1.1726	2.4331E-01	7.5844E-01
5-KETE	Oxylipin	0.2115	0.1803	1.1730	2.4342E-01	7.5844E-01
HomoCys	Amine	-0.1708	0.1480	-1.1546	2.5042E-01	7.6135E-01
LPA (18:1)	Lysophospholipid	-0.2112	0.1831	-1.1537	2.5103E-01	7.6135E-01
16-HDoHE/DHA	Oxylipin	0.2370	0.2075	1.1418	2.5569E-01	7.6135E-01
w3FA/w6FA	Fatty acid	0.1360	0.1192	1.1411	2.5605E-01	7.6135E-01
LCA	Bile Acid	-0.2173	0.1907	-1.1398	2.5721E-01	7.6135E-01
Sum PBA	Bile Acid	0.2301	0.2044	1.1256	2.6263E-01	7.6424E-01
Ornithine/Arg	Amine	0.2286	0.2031	1.1258	2.6335E-01	7.6424E-01
15-HETrE	Oxylipin	0.2071	0.1861	1.1128	2.6858E-01	7.6586E-01
8,12-iso-iPF2alpha-VI/AA	Oxylipin	-0.2089	0.1883	-1.1089	2.6999E-01	7.6586E-01
13,14-dihydro-15-keto-PGF2alpha	Oxylipin	-0.1929	0.1752	-1.1008	2.7385E-01	7.6586E-01
5-HETE	Oxylipin	-0.2034	0.1849	-1.0997	2.7426E-01	7.6586E-01
S1P (16:1)	Lysophospholipid	-0.1605	0.1509	-1.0638	2.8959E-01	7.9424E-01
LPE (18:1)	Lysophospholipid	-0.1618	0.1535	-1.0540	2.9410E-01	7.9424E-01
15-HETE/AA	Oxylipin	0.1969	0.1877	1.0491	2.9643E-01	7.9424E-01
TUDCA	Bile Acid	0.2200	0.2101	1.0470	2.9748E-01	7.9424E-01
g-Glu-Gln	Amine	-0.2078	0.1987	-1.0456	2.9784E-01	7.9424E-01
12-KETE	Oxylipin	0.2132	0.2083	1.0233	3.0816E-01	8.1444E-01
TXB3/EPA	Oxylipin	-0.1662	0.1672	-0.9941	3.2255E-01	8.3805E-01
5-HETE/AA	Oxylipin	-0.1885	0.1898	-0.9929	3.2276E-01	8.3805E-01
LPE (22:4)	Lysophospholipid	-0.1521	0.1561	-0.9744	3.3183E-01	8.4756E-01
LPI (16:1)	Lysophospholipid	0.1842	0.1905	0.9671	3.3547E-01	8.4756E-01
13-HDoHE/DHA	Oxylipin	0.1937	0.2005	0.9662	3.3578E-01	8.4756E-01
Asp	Amine	0.1922	0.1997	0.9627	3.3831E-01	8.4756E-01
EPA	Fatty acid	0.1131	0.1181	0.9570	3.4074E-01	8.4756E-01
16-HDoHE	Oxylipin	0.1571	0.1673	0.9388	3.4998E-01	8.6327E-01
PAF 16(0)	PAF	-0.2009	0.2176	-0.9231	3.5781E-01	8.7404E-01
Kyn/Trp	Amine	0.2015	0.2192	0.9188	3.6025E-01	8.7404E-01
LPS (18:1)	Lysophospholipid	-0.1830	0.2003	-0.9133	3.6352E-01	8.7481E-01
PGE1	Oxylipin	0.1872	0.2082	0.8988	3.7093E-01	8.8543E-01
12-KETE/12-HETE	Oxylipin	0.1776	0.2010	0.8837	3.7855E-01	8.8543E-01
cLPA (18:0)	Lysophospholipid	0.1651	0.1868	0.8836	3.7871E-01	8.8543E-01
9-HODE	Oxylipin	0.1678	0.1912	0.8773	3.8235E-01	8.8543E-01
HCA	Bile Acid	0.1627	0.1858	0.8756	3.8289E-01	8.8543E-01
AABA	Amine	0.1719	0.2001	0.8592	3.9204E-01	8.9669E-01
LPS (22:6)	Lysophospholipid	0.1281	0.1500	0.8539	3.9505E-01	8.9669E-01
Anserine	Amine	0.1765	0.2079	0.8487	3.9827E-01	8.9669E-01
Carnosine	Amine	-0.1409	0.1668	-0.8448	3.9987E-01	8.9669E-01
19,20-EpDPE/DHA	Oxylipin	0.1695	0.2021	0.8386	4.0329E-01	8.9755E-01
Clupanodonic acid	Fatty acid	0.1325	0.1598	0.8290	4.0903E-01	8.9776E-01
15-HEPE	Oxylipin	0.1491	0.1800	0.8280	4.0945E-01	8.9776E-01
GCDA	Bile Acid	0.1286	0.1593	0.8072	4.2101E-01	8.9893E-01
LPA (16:1)	Lysophospholipid	-0.1294	0.1603	-0.8071	4.2131E-01	8.9893E-01
LPA (18:2)	Lysophospholipid	-0.1362	0.1693	-0.8045	4.2279E-01	8.9893E-01
19,20-EpDPE	Oxylipin	0.1753	0.2188	0.8011	4.2462E-01	8.9893E-01
GLA	Fatty acid	-0.1501	0.1893	-0.7927	4.2973E-01	8.9893E-01
Lys	Amine	-0.1396	0.1763	-0.7920	4.2995E-01	8.9893E-01
Tau	Amine	-0.1527	0.1939	-0.7876	4.3243E-01	8.9893E-01
delta-17,6-keto-PGF1alpha/EPA	Oxylipin	0.1378	0.1755	0.7852	4.3428E-01	8.9893E-01

Diagnosis of Late-Onset Sepsis

SDMA	Amine	-0.1355	0.1746	-0.7762	4.3932E-01	9.0039E-01
FA (16:0)	Fatty acid	-0.1575	0.2047	-0.7692	4.4361E-01	9.0039E-01
12,13-EpOME	Oxylipin	-0.1489	0.1957	-0.7610	4.4831E-01	9.0039E-01
ETE	Fatty acid	-0.1513	0.2013	-0.7515	4.5405E-01	9.0039E-01
2-aminoadipic acid	Amine	-0.1279	0.1717	-0.7447	4.5782E-01	9.0039E-01
Pro	Amine	0.1578	0.2121	0.7437	4.5865E-01	9.0039E-01
Ile	Amine	-0.1590	0.2162	-0.7352	4.6371E-01	9.0039E-01
Sum iPs	Oxylipin	0.1173	0.1605	0.7313	4.6605E-01	9.0039E-01
3-Methoxy-tyramine	Amine	0.1590	0.2175	0.7309	4.6689E-01	9.0039E-01
13-HDoHE	Oxylipin	0.1254	0.1719	0.7293	4.6747E-01	9.0039E-01
9-HEPE/EPA	Oxylipin	-0.1255	0.1743	-0.7204	4.7288E-01	9.0039E-01
LPG (20:4)	Lysophospholipid	-0.1216	0.1712	-0.7099	4.7911E-01	9.0039E-01
11-HETE/AA	Oxylipin	0.1310	0.1864	0.7028	4.8354E-01	9.0039E-01
19,20-DiHDDPA	Oxylipin	0.1409	0.2011	0.7006	4.8504E-01	9.0039E-01
DGLA	Fatty acid	0.1413	0.2027	0.6971	4.8730E-01	9.0039E-01
LPA (16:0)	Lysophospholipid	-0.1146	0.1668	-0.6870	4.9345E-01	9.0039E-01
AA	Fatty acid	-0.1390	0.2032	-0.6843	4.9533E-01	9.0039E-01
12,13-DiHOME	Oxylipin	0.0807	0.1189	0.6790	4.9869E-01	9.0039E-01
8-HDoHE/DHA	Oxylipin	0.1366	0.2039	0.6700	5.0408E-01	9.0039E-01
Sum HETEs	Oxylipin	-0.1218	0.1824	-0.6675	5.0600E-01	9.0039E-01
Gly-Gly	Amine	0.1186	0.1780	0.6666	5.0669E-01	9.0039E-01
Sum HODEs	Oxylipin	0.1265	0.1900	0.6656	5.0723E-01	9.0039E-01
5-aminolevulinic acid	Amine	-0.1220	0.1836	-0.6646	5.0747E-01	9.0039E-01
9-KODE	Oxylipin	0.1207	0.1860	0.6490	5.1769E-01	9.0039E-01
PGA2	Oxylipin	-0.1204	0.1856	-0.6486	5.1790E-01	9.0039E-01
Citrulline/Ornithine	Amine	-0.1037	0.1606	-0.6456	5.2000E-01	9.0039E-01
5-IPF2alpha-VI	Oxylipin	-0.1115	0.1739	-0.6411	5.2297E-01	9.0039E-01
PGE2/AA	Oxylipin	0.1273	0.1993	0.6390	5.2419E-01	9.0039E-01
Kyn	Amine	-0.1302	0.2048	-0.6357	5.2629E-01	9.0039E-01
cLPA (20:4)	Lysophospholipid	-0.1194	0.1883	-0.6338	5.2761E-01	9.0039E-01
15-HETE/DGLA	Oxylipin	0.1208	0.1937	0.6235	5.3426E-01	9.0039E-01
FA (18:0)	Fatty acid	-0.1276	0.2058	-0.6201	5.3657E-01	9.0039E-01
8-HDoHE	Oxylipin	0.1057	0.1706	0.6197	5.3679E-01	9.0039E-01
LPE (20:5)	Lysophospholipid	-0.1133	0.1836	-0.6171	5.3841E-01	9.0039E-01
LPG (22:4)	Lysophospholipid	-0.1206	0.1980	-0.6088	5.4375E-01	9.0422E-01
18-HEPE	Oxylipin	0.0965	0.1645	0.5866	5.5885E-01	9.1828E-01
TXB1	Oxylipin	0.1006	0.1748	0.5759	5.6591E-01	9.1828E-01
11beta-PGF2alpha/AA	Oxylipin	0.0940	0.1635	0.5750	5.6634E-01	9.1828E-01
Sum PGs	Oxylipin	0.1159	0.2062	0.5623	5.7505E-01	9.1828E-01
Gln	Amine	-0.1119	0.1997	-0.5606	5.7611E-01	9.1828E-01
Cystathionine	Amine	-0.0843	0.1516	-0.5563	5.7899E-01	9.1828E-01
20-HETE	Oxylipin	-0.1139	0.2050	-0.5554	5.7975E-01	9.1828E-01
17-HDoHE/DHA	Oxylipin	0.1130	0.2038	0.5543	5.8041E-01	9.1828E-01
PAF 18(2)	PAF	0.0984	0.1785	0.5512	5.8248E-01	9.1828E-01
Ser	Amine	-0.1079	0.1960	-0.5505	5.8323E-01	9.1828E-01
Sum LG	Endocannabinoid	0.0910	0.1679	0.5421	5.8888E-01	9.2227E-01
AdA	Fatty acid	-0.1054	0.1969	-0.5354	5.9340E-01	9.2442E-01
7-HDoHE	Oxylipin	0.0904	0.1702	0.5310	5.9650E-01	9.2442E-01
Leu	Amine	-0.1089	0.2084	-0.5224	6.0246E-01	9.2879E-01
LPG (22:6)	Lysophospholipid	0.0685	0.1329	0.5156	6.0720E-01	9.3002E-01
11,12-EpETE	Oxylipin	-0.0826	0.1646	-0.5021	6.1675E-01	9.3002E-01
LPI (22:6)	Lysophospholipid	0.0951	0.1911	0.4976	6.1980E-01	9.3002E-01
9-HpODE/LA	Oxylipin	-0.0853	0.1714	-0.4975	6.1988E-01	9.3002E-01
His	Amine	-0.0860	0.1730	-0.4968	6.2040E-01	9.3002E-01
7-HDoHE/DHA	Oxylipin	0.0974	0.1978	0.4923	6.2336E-01	9.3002E-01
Sum AG	Endocannabinoid	0.0937	0.1920	0.4881	6.2646E-01	9.3002E-01
18-HEPE/EPA	Oxylipin	-0.0848	0.1767	-0.4799	6.3232E-01	9.3002E-01
PGF1alpha	Oxylipin	0.0759	0.1591	0.4770	6.3419E-01	9.3002E-01
GCA	Bile Acid	-0.0932	0.1958	-0.4763	6.3468E-01	9.3002E-01
THDCA	Bile Acid	-0.0680	0.1441	-0.4718	6.3795E-01	9.3022E-01
9-HpODE	Oxylipin	0.0760	0.1639	0.4634	6.4406E-01	9.3277E-01
13,14-dihydro-15-keto-PGF2alpha/AA	Oxylipin	-0.0903	0.1971	-0.4583	6.4771E-01	9.3277E-01
BCAA	Amine	-0.0910	0.2010	-0.4525	6.5178E-01	9.3277E-01
Coriolic acid	Oxylipin	0.0821	0.1884	0.4359	6.6387E-01	9.3277E-01
17-HDoHE	Oxylipin	0.0799	0.1835	0.4355	6.6416E-01	9.3277E-01
20-HDoHE/DHA	Oxylipin	0.0807	0.1887	0.4274	6.6990E-01	9.3277E-01
8-iso-PGF3alpha/DGLA	Oxylipin	0.0641	0.1519	0.4219	6.7377E-01	9.3277E-01
10-HDoHE/DHA	Oxylipin	-0.0832	0.1975	-0.4213	6.7444E-01	9.3277E-01
TXB3	Oxylipin	-0.0708	0.1683	-0.4206	6.7487E-01	9.3277E-01
12-HEPE	Oxylipin	0.0736	0.1775	0.4149	6.7913E-01	9.3277E-01
LPI (22:4)	Lysophospholipid	-0.0723	0.1752	-0.4127	6.8052E-01	9.3277E-01
9-KODE/9-HODE	Oxylipin	-0.0770	0.1887	-0.4082	6.8395E-01	9.3277E-01
cLPA (18:2)	Lysophospholipid	0.0721	0.1782	0.4044	6.8669E-01	9.3277E-01
14-HDoHE/DHA	Oxylipin	-0.0777	0.1939	-0.4009	6.8937E-01	9.3277E-01

Chapter III

PGA2/AA	Oxylipin	-0.0762	0.1908	-0.3992	6.9047E-01	9.3277E-01
O-Acetyl-Ser	Amine	-0.0739	0.1854	-0.3989	6.9060E-01	9.3277E-01
Ala	Amine	-0.0790	0.2027	-0.3900	6.9726E-01	9.3277E-01
20-HDoHE	Oxylipin	0.0737	0.1890	0.3898	6.9751E-01	9.3277E-01
PGE1/DGLA	Oxylipin	0.0784	0.2031	0.3861	7.0025E-01	9.3277E-01
14-HDoHE	Oxylipin	-0.0822	0.2148	-0.3828	7.0273E-01	9.3277E-01
8-HETE	Oxylipin	0.0696	0.1899	0.3668	7.1460E-01	9.4429E-01
LPG (18:1)	Lysophospholipid	-0.0746	0.2107	-0.3540	7.2397E-01	9.4637E-01
Gln/Glu	Amine	-0.0771	0.2195	-0.3514	7.2601E-01	9.4637E-01
11-HDoHE/DHA	Oxylipin	0.0700	0.2010	0.3484	7.2823E-01	9.4637E-01
cLPA (18:1)	Lysophospholipid	-0.0593	0.1727	-0.3434	7.3198E-01	9.4637E-01
PGF2alpha	Oxylipin	0.0668	0.1991	0.3353	7.3804E-01	9.4637E-01
O-PO3-EA	Amine	-0.0712	0.2140	-0.3327	7.4001E-01	9.4637E-01
Sum TXs	Oxylipin	-0.0567	0.1706	-0.3323	7.4031E-01	9.4637E-01
9-HEPE	Oxylipin	0.0533	0.1614	0.3305	7.4175E-01	9.4637E-01
Glutathione	Amine	-0.0540	0.1775	-0.3042	7.6145E-01	9.5411E-01
AEA	Endocannabinoid	0.0437	0.1437	0.3043	7.6163E-01	9.5411E-01
15-HETE	Oxylipin	0.0562	0.1944	0.2889	7.7326E-01	9.5411E-01
Cystathionine/HomoCys	Amine	0.0464	0.1611	0.2882	7.7362E-01	9.5411E-01
beta-Ala	Amine	-0.0544	0.1939	-0.2804	7.7964E-01	9.5411E-01
12-HETE	Oxylipin	-0.0554	0.1979	-0.2797	7.8027E-01	9.5411E-01
Ornithine	Amine	-0.0523	0.1905	-0.2747	7.8408E-01	9.5411E-01
LPG (18:3)	Lysophospholipid	0.0271	0.1553	0.2741	7.8449E-01	9.5411E-01
9-HOTrE/ALA	Oxylipin	-0.0503	0.1854	-0.2714	7.8658E-01	9.5411E-01
10-HDoHE	Oxylipin	-0.0530	0.1981	-0.2673	7.8978E-01	9.5411E-01
8-iso-PGF3alpha	Oxylipin	0.0379	0.1427	0.2658	7.9086E-01	9.5411E-01
LPE (18:3)	Lysophospholipid	-0.0422	0.1590	-0.2651	7.9145E-01	9.5411E-01
LPG (18:0)	Lysophospholipid	0.0492	0.1903	0.2588	7.9629E-01	9.5411E-01
11beta-PGF2alpha	Oxylipin	0.0374	0.1485	0.2523	8.0132E-01	9.5411E-01
TCA	Bile Acid	-0.0437	0.1736	-0.2520	8.0155E-01	9.5411E-01
9-HODE/9-HpODE	Oxylipin	0.0490	0.1952	0.2510	8.0226E-01	9.5411E-01
Cys/Cystathionine	Amine	0.0449	0.1819	0.2468	8.0544E-01	9.5411E-01
LPA (14:0)	Lysophospholipid	0.0342	0.1389	0.2464	8.0583E-01	9.5411E-01
Phe	Amine	-0.0455	0.1895	-0.2403	8.1065E-01	9.5599E-01
Sum SBA	Bile Acid	0.0511	0.2184	0.2338	8.1557E-01	9.5797E-01
Glu	Amine	0.0445	0.2124	0.2096	8.3444E-01	9.6298E-01
19,20-DiHDPA/19,20-EpDPE	Oxylipin	-0.0429	0.2049	-0.2093	8.3459E-01	9.6298E-01
Sum HDoHEs	Oxylipin	-0.0426	0.2051	-0.2079	8.3579E-01	9.6298E-01
11-HDoHE	Oxylipin	0.0393	0.1942	0.2024	8.3998E-01	9.6298E-01
5-IPF2alpha-VI/AA	Oxylipin	-0.0361	0.1859	-0.1941	8.4647E-01	9.6298E-01
PGF1alpha/DGLA	Oxylipin	0.0329	0.1709	0.1925	8.4768E-01	9.6298E-01
Sarcosine	Amine	-0.0379	0.1979	-0.1917	8.4829E-01	9.6298E-01
S1P (18:0)	Lysophospholipid	0.0358	0.1927	0.1858	8.5292E-01	9.6298E-01
3-Met-His	Amine	0.0378	0.2068	0.1825	8.5550E-01	9.6298E-01
LPA (18:0)	Lysophospholipid	-0.0329	0.1803	-0.1824	8.5559E-01	9.6298E-01
15-HEPE/EPA	Oxylipin	0.0321	0.1771	0.1813	8.5642E-01	9.6298E-01
LPG (20:3)	Lysophospholipid	0.0386	0.2164	0.1782	8.5888E-01	9.6298E-01
Cys	Amine	-0.0261	0.1583	-0.1651	8.6916E-01	9.7084E-01
11,12-EpETrE/AA	Oxylipin	0.0308	0.2028	0.1521	8.7936E-01	9.7542E-01
ALA	Fatty acid	0.0178	0.1242	0.1433	8.8634E-01	9.7542E-01
20-HETE/AA	Oxylipin	-0.0269	0.1910	-0.1408	8.8835E-01	9.7542E-01
Sum HEPEs	Oxylipin	0.0230	0.1674	0.1376	8.9080E-01	9.7542E-01
PGE2	Oxylipin	0.0299	0.2177	0.1372	8.9115E-01	9.7542E-01
TXB2/AA	Oxylipin	0.0226	0.1719	0.1318	8.9542E-01	9.7542E-01
Val	Amine	-0.0226	0.1853	-0.1220	9.0311E-01	9.7542E-01
DHA	Fatty acid	0.0187	0.1579	0.1184	9.0599E-01	9.7542E-01
12-HHTrE	Oxylipin	-0.0190	0.1638	-0.1157	9.0809E-01	9.7542E-01
LPG (16:1)	Lysophospholipid	-0.0221	0.1927	-0.1148	9.0880E-01	9.7542E-01
12-HEPE/EPA	Oxylipin	-0.0208	0.1892	-0.1101	9.1258E-01	9.7542E-01
12-HHTrE/AA	Oxylipin	0.0180	0.1636	0.1097	9.1281E-01	9.7542E-01
Arg/ADMA	Amine	-0.0193	0.1876	-0.1031	9.1810E-01	9.7606E-01
Gly	Amine	0.0170	0.1756	0.0969	9.2296E-01	9.7606E-01
12-HETE/AA	Oxylipin	0.0188	0.1943	0.0965	9.2330E-01	9.7606E-01
TXBI/DGLA	Oxylipin	0.0139	0.1724	0.0807	9.3589E-01	9.8369E-01
11-HETE	Oxylipin	0.0145	0.1831	0.0790	9.3717E-01	9.8369E-01
TLCA-3S	Bile Acid	-0.0149	0.2015	-0.0741	9.4105E-01	9.8428E-01
8-HETrE/DGLA	Oxylipin	-0.0127	0.1909	-0.0667	9.4693E-01	9.8548E-01
5-HEPE	Oxylipin	0.0112	0.1917	0.0585	9.5344E-01	9.8548E-01
Sum HETrEs	Oxylipin	0.0094	0.1836	0.0514	9.5909E-01	9.8548E-01
LPG (18:2)	Lysophospholipid	0.0082	0.1712	0.0482	9.6165E-01	9.8548E-01
9-HOTrE	Oxylipin	-0.0079	0.1784	-0.0443	9.6477E-01	9.8548E-01
cLPA (14:0)	Lysophospholipid	-0.0048	0.1483	-0.0323	9.7429E-01	9.8548E-01
EA	Amine	-0.0057	0.1763	-0.0322	9.7435E-01	9.8548E-01
LPI (20:4)	Lysophospholipid	-0.0055	0.1728	-0.0317	9.7474E-01	9.8548E-01

LPA (20:5)	Lysophospholipid	0.0051	0.1626	0.0311	9.7524E-01	9.8548E-01
LPS (18:2)	Lysophospholipid	0.0054	0.1754	0.0308	9.7550E-01	9.8548E-01
3-AIBA	Amine	-0.0038	0.1500	-0.0256	9.7962E-01	9.8624E-01
LPA (22:5)	Lysophospholipid	0.0035	0.1784	0.0197	9.8435E-01	9.8624E-01
TXB2	Oxylipin	-0.0029	0.1703	-0.0173	9.8624E-01	9.8624E-01

Table S7: Raw fold change values and corresponding linear mixed-effect model p-values of highlighted metabolites

Insignificant fold change (technical variation higher than fold change)

Etiology-independent metabolic signatures of systemic inflammation						
Metabolite	C-SSI FC	C SSI p-value	C-S FC	C S p-value	SSI-S FC	SSI S p-value
Gly	0.9	3.9492E-03	0.87	1.5106E-03	0.96	9.2296E-01
Gln	0.75	7.2418E-05	0.74	4.5579E-06	0.98	5.7611E-01
Lys	0.9	1.3971E-02	0.82	5.2260E-05	0.91	4.2995E-01
Ser	0.86	2.2684E-03	0.82	3.1483E-04	0.95	5.8323E-01
His	0.86	5.6806E-03	0.85	2.7890E-04	0.99	6.2040E-01
Saccharopine	0.72	1.8606E-03	0.75	1.5333E-03	1.05	1.0201E-01
Ornithine	0.81	2.9195E-04	0.79	8.8819E-05	0.98	7.8408E-01
BCAA	0.91	2.3484E-02	0.9	1.0572E-03	0.99	6.5178E-01
5,6-DiHETrE	0.58	1.5236E-02	0.55	8.3038E-04	0.94	1.8593E-01
8,9-DiHETrE	0.61	8.7321E-03	0.62	2.5211E-04	1.02	1.7108E-01
11,12-DiHETrE	0.62	4.6377E-02	0.58	3.6048E-03	0.93	4.9231E-02
5-HETE	0.77	2.3464E-02	0.73	2.2557E-02	0.95	2.7426E-01
S1P (16:1)	0.77	1.7291E-01	0.73	1.2206E-02	0.95	2.8959E-01
S1P (18:1)	0.8	1.2630E-01	0.79	7.6709E-03	0.98	2.0974E-01
LPE (16:1)	0.78	2.1974E-01	0.71	4.2831E-02	0.92	1.6101E-01
LPE (18:2)	0.82	1.4706E-01	0.83	6.3655E-03	1.01	2.1971E-01
LPE (20:3)	0.75	8.8873E-02	0.74	1.3460E-03	0.98	1.6295E-01
LPE (20:5)	0.88	1.4716E-01	0.89	1.4725E-02	1.02	5.3841E-01
LPE (22:4)	0.75	1.2473E-01	0.68	1.2747E-04	0.91	3.3183E-01
LPE (22:6)	0.83	6.0592E-02	0.8	1.2898E-04	0.96	1.2492E-01
PGE2	1.18	1.5481E-01	1.34	8.2617E-03	1.14	8.7389E-01
5-HETE/AA	0.77	6.4588E-03	0.79	3.8870E-03	1.04	3.2276E-01
g-Glu-Gln	0.68	3.0942E-04	0.71	4.5095E-05	1.05	2.9784E-01
cLPA (16:1)	0.82	9.9418E-03	0.8	4.7459E-04	0.97	1.0361E-01
Gln/Glu	0.81	6.1041E-03	0.76	1.4586E-03	0.94	7.2601E-01
Ile	0.9	2.3631E-02	0.86	1.2120E-04	0.96	4.6371E-01
Ala	0.93	1.2453E-01	0.89	8.4215E-03	0.95	6.9726E-01
cLPA (14:0)	0.81	1.0135E-02	0.82	7.8417E-03	1.01	9.7429E-01
Leu	0.92	6.1352E-02	0.91	1.8036E-03	0.98	6.0246E-01
Val	0.91	2.4882E-02	0.92	8.8328E-03	1.01	9.0311E-01

Metabolic markers of enhanced immune dysregulation in sepsis						
Metabolite	C-SSI FC	C SSI p-value	C-S FC	C S p-value	SSI-S FC	SSI S p-value
Cortisol	2.41	6.2885E-03	3.61	2.0526E-09	1.5	1.7202E-01
LPS (18:0)	1.67	4.6607E-05	2.16	2.2959E-10	1.29	3.6274E-02
LPI (18:0)	1.11	4.5811E-02	1.37	5.5238E-08	1.23	6.4725E-03
PGE1	1.16	2.1461E-01	1.52	1.9932E-03	1.31	4.2768E-01
5-HT/Trp	1.22	4.6230E-02	3.53	1.7823E-06	2.88	1.2361E-03
Phe/Tyr	1.22	3.0388E-01	1.29	1.5184E-08	1.05	4.3180E-04
Trp	0.78	2.0105E-05	0.71	3.4127E-11	0.91	8.3957E-03
Thr	0.83	9.5501E-04	0.71	1.5413E-09	0.85	5.5925E-03
Arg	0.79	6.1110E-02	0.67	9.1560E-07	0.84	3.6136E-02
Met	0.9	4.2360E-02	0.81	2.4988E-06	0.9	1.8160E-01
Tyr	0.87	2.8915E-01	0.68	2.2626E-06	0.79	4.0870E-03
3-Methoxy-tyrosine	0.91	3.7489E-01	0.75	4.3945E-05	0.82	1.0768E-02
OH-Lys	0.86	9.4594E-03	0.76	1.6084E-08	0.88	2.9776E-03
4-OH-Pro	0.86	6.8759E-03	0.74	4.0514E-09	0.86	3.5451E-03
4-OH-Pro/Pro	0.88	1.2024E-01	0.74	7.3099E-08	0.84	1.8963E-04
Sum OG	0.85	2.9301E-03	0.78	6.1609E-04	0.92	2.0130E-01
S1P (18:2)	0.76	1.5521E-02	0.7	8.6977E-06	0.92	3.6966E-02
AAA	0.91	1.4582E-01	0.78	1.9771E-06	0.85	9.2794E-03

Sepsis-specific metabolic dysregulation beyond inflammation						
Metabolite	C-SSI FC	C SSI p-value	C-S FC	C S p-value	SSI-S FC	SSI S p-value
LPE (16:0)	1.02	2.4789E-01	1.2	1.8889E-05	1.17	4.4790E-03
LPE (18:0)	0.98	9.2321E-01	1.13	1.6971E-03	1.15	8.9408E-03
LPI (16:0)	1.07	3.2484E-01	1.35	8.9704E-06	1.26	9.8549E-04

Chapter III

LPS (16:0)	1	8.9890E-01	1.04	1.9731E-03	1.03	2.6221E-02
DHEA	1.02	7.1005E-01	1.12	6.0580E-04	1.11	1.1767E-01
Sum KETEs	1.18	5.1535E-01	1.32	5.6095E-03	1.12	1.4701E-01
Citrulline	0.98	8.4429E-01	0.83	7.2990E-05	0.86	2.0050E-01
Homoserine	1.01	5.6101E-01	0.89	8.0334E-03	0.88	2.7817E-02
Trimethyl-Lys	1	4.8874E-01	0.95	2.9736E-03	0.95	3.0060E-02
5-HT	0.8	3.4914E-01	2.27	1.4946E-03	2.83	1.5204E-02
Arg/Lys	0.89	8.0096E-01	0.82	2.4128E-03	0.93	7.6968E-02
Putrescine	1.17	9.0351E-01	1.69	8.1280E-03	1.45	1.6671E-03
Sphinganine18.0	0.92	6.3327E-01	1.04	3.9278E-02	1.13	8.4047E-03
Sphingosine18.1	0.93	8.5370E-01	1	2.1940E-02	1.08	6.7077E-02
BCAA/AAA	1	2.2707E-01	1.13	2.3564E-02	1.13	3.8189E-03
Oleic acid	0.98	3.8532E-01	0.95	2.0778E-02	0.97	1.2792E-01
1-Met-His	0.99	5.3502E-01	0.96	6.6580E-03	0.97	1.9998E-02

Table S8: Linear mixed-effect model results of the blood culture-stratified "Sepsis" models

Metabolite	Estimate Culture-Negative	Estimate Culture-Positive	Standard Error Culture-Negative	Standard Error Culture-Positive	p-value Culture-Negative	p-value Culture-Positive	Adjusted p-value Culture-Negative	Adjusted p-value Culture-Positive
LPI (18:0)	0.9519	0.5602	0.1663	0.1547	4.6206E-08	3.9403E-04	1.3677E-05	4.6654E-03
4-OH-Pro/Pro	-0.8970	-0.4882	0.1723	0.1645	5.5777E-07	3.4223E-03	8.2550E-05	2.0260E-02
LPI (16:0)	0.8763	0.5484	0.1768	0.1707	1.7206E-06	1.5726E-03	1.3182E-04	1.2514E-02
5-HT/Trp	0.9293	0.6441	0.1878	0.1766	1.7814E-06	3.5585E-04	1.3182E-04	4.3888E-03
4-OH-Pro	-0.7876	-0.7275	0.1643	0.1584	3.5077E-06	8.4579E-06	2.0765E-04	3.1294E-04
5-HT	0.8001	0.3696	0.1863	0.1784	2.9202E-05	3.9834E-02	1.4252E-03	1.2156E-01
Cortisol	0.7750	0.5189	0.1819	0.1699	3.3704E-05	2.6250E-03	1.4252E-03	1.6946E-02
LPS (18:0)	0.7460	0.8796	0.1790	0.1632	4.9620E-05	2.3721E-07	1.8359E-03	3.5107E-05
OH-Lys	-0.6988	-0.7500	0.1748	0.1656	9.4481E-05	1.1176E-05	3.1074E-03	3.6755E-04
Thr	-0.5999	-0.7934	0.1545	0.1498	1.4868E-04	3.5916E-07	4.4009E-03	3.5437E-05
LPI (18:1)	0.6654	0.2211	0.1749	0.1672	2.0003E-04	1.8786E-01	5.3826E-03	3.9160E-01
PGF1alpha	-0.5420	0.2288	0.1451	0.1111	2.5487E-04	4.1064E-02	6.2867E-03	1.2403E-01
LPE (16:0)	0.5553	0.6063	0.1582	0.1590	5.7183E-04	1.9222E-04	1.3020E-02	2.7094E-03
Phe/Tyr	0.4147	0.5817	0.1211	0.1200	7.6903E-04	2.7689E-06	1.6259E-02	1.2595E-04
Gly-Pro	-0.5537	-0.5180	0.1671	0.1546	1.1254E-03	9.9091E-04	2.2209E-02	9.4143E-03
LPS (22:4)	0.6188	0.3138	0.1927	0.1791	1.5749E-03	8.1527E-02	2.9135E-02	2.0803E-01
LPS (16:0)	0.5924	0.1216	0.1912	0.1879	2.2747E-03	5.1838E-01	3.9606E-02	6.7894E-01
Carnosine	-0.4550	-0.0512	0.1492	0.1450	2.6530E-03	7.2453E-01	4.3628E-02	8.6826E-01
OH-Lys/Lys	-0.5409	-0.1425	0.1809	0.1718	3.1929E-03	4.0794E-01	4.7245E-02	5.9482E-01
11,12-EpETE/AA	-0.5406	-0.1194	0.1808	0.1722	3.2107E-03	4.8896E-01	4.7245E-02	6.6391E-01
LPI (16:1)	0.5346	-0.0334	0.1796	0.1759	3.3519E-03	8.4951E-01	4.7245E-02	9.3826E-01
PGF1alpha/DGLA	-0.4641	0.2170	0.1583	0.1478	3.8715E-03	1.4373E-01	5.1431E-02	3.1987E-01
Sphingosine18.1	0.5859	0.2340	0.2009	0.1947	4.0165E-03	2.3117E-01	5.1431E-02	4.3035E-01
3-Methoxytyrosine	-0.5061	-0.6180	0.1743	0.1600	4.1701E-03	1.5828E-04	5.1431E-02	2.5809E-03
LPG (16:0)	0.5207	-0.1109	0.1816	0.1840	4.6559E-03	5.4751E-01	5.5125E-02	7.0462E-01
Trp	-0.4011	-0.8270	0.1409	0.1403	4.9445E-03	2.0752E-08	5.6292E-02	6.1427E-06
PGE1	0.5263	0.3897	0.1889	0.1993	5.9626E-03	5.2259E-02	6.5368E-02	1.4902E-01
Gly-Gly	0.4674	-0.0811	0.1684	0.1585	6.2337E-03	6.0954E-01	6.5899E-02	7.5491E-01
LPI (14:0)	0.4058	-0.0992	0.1490	0.1508	7.1268E-03	5.1173E-01	7.2743E-02	6.7321E-01
SIP (18:2)	-0.3739	-0.5589	0.1423	0.1455	9.4004E-03	1.7439E-04	9.2751E-02	2.5809E-03
Anserine	-0.4296	0.1616	0.1652	0.1857	1.0123E-02	3.8533E-01	9.4437E-02	5.7604E-01
LPE (18:0)	0.4087	0.4534	0.1573	0.1487	1.0209E-02	2.6640E-03	9.4437E-02	1.6946E-02
LPG (18:0)	0.4302	-0.0127	0.1679	0.1715	1.1250E-02	9.4124E-01	1.0090E-01	9.9614E-01
Asp	0.4831	-0.0594	0.1906	0.1900	1.2241E-02	7.5480E-01	1.0657E-01	8.6862E-01
8-iso-PGF3alpha	-0.3200	-0.0063	0.1275	0.1275	1.3385E-02	9.6091E-01	1.1320E-01	9.9764E-01
PGF2alpha	0.4725	0.3010	0.1997	0.1919	1.9129E-02	1.1861E-01	1.5430E-01	2.7863E-01
S-Methyl-Cys	-0.4126	-0.4289	0.1747	0.1729	1.9288E-02	1.4099E-02	1.5430E-01	5.7168E-02
ADMA	-0.4302	-0.8076	0.1834	0.1670	2.0201E-02	2.9786E-06	1.5557E-01	1.2595E-04
DEA	0.4617	0.2501	0.1972	0.1921	2.0497E-02	1.9479E-01	1.5557E-01	3.9765E-01
LPE (22:4)	-0.3781	-0.4077	0.1640	0.1575	2.2337E-02	1.0447E-02	1.6220E-01	4.5474E-02
LPS (22:6)	0.3234	0.1895	0.1404	0.1290	2.2467E-02	1.4359E-01	1.6220E-01	3.1987E-01
LPG (22:6)	0.2854	0.0267	0.1280	0.1119	2.7065E-02	8.1156E-01	1.8594E-01	9.0650E-01
18-HEPE	0.3859	0.2131	0.1731	0.1702	2.7163E-02	2.1236E-01	1.8594E-01	4.1013E-01
LPI (22:6)	0.3837	-0.1162	0.1727	0.1876	2.7643E-02	5.3654E-01	1.8594E-01	6.9656E-01
EPA	0.2411	0.0831	0.1090	0.1062	2.8268E-02	4.3517E-01	1.8594E-01	6.1632E-01
LPE (20:4)	-0.3590	-0.5052	0.1647	0.1609	3.0693E-02	1.9864E-03	1.9168E-01	1.3725E-02
Sphinganine18.0	0.4194	0.5259	0.1928	0.1944	3.0937E-02	7.5281E-03	1.9168E-01	3.7109E-02
13,14-dihydro-15-keto-PGF2alpha/AA	-0.4179	0.1838	0.1922	0.1761	3.1083E-02	2.9822E-01	1.9168E-01	4.9842E-01
Sum KETEs	0.4198	0.4101	0.1954	0.1890	3.1313E-02	3.1404E-02	2.0014E-01	1.0563E-01

Diagnosis of Late-Onset Sepsis

Gln/Glu	-0.4152	-0.5236	0.1955	0.1965	3.5134E-02	8.4997E-03	2.0799E-01	3.9683E-02
Gln	-0.3904	-0.6981	0.1864	0.1812	3.7702E-02	1.6600E-04	2.0887E-01	2.5809E-03
5-HETE/AA	-0.3474	-0.4129	0.1659	0.1628	3.7787E-02	1.2098E-02	2.0887E-01	4.9736E-02
8-iso-PGF3alpha/DGLA	-0.3202	0.0252	0.1530	0.1497	3.8097E-02	8.6658E-01	2.0887E-01	9.4865E-01
Tyr	-0.2964	-0.6861	0.1418	0.1392	3.8105E-02	1.9211E-06	2.0887E-01	1.1373E-04
LPI (18:2)	0.3012	0.1088	0.1457	0.1402	4.0307E-02	4.3847E-01	2.0956E-01	6.1804E-01
14,15-DiHETE	0.3444	0.0818	0.1667	0.1529	4.0472E-02	5.9336E-01	2.0956E-01	7.4421E-01
Ser	-0.3787	-0.4888	0.1839	0.1842	4.1062E-02	8.7209E-03	2.0956E-01	3.9683E-02
LPG (14:0)	0.2619	-0.3127	0.1272	0.1181	4.1063E-02	8.8482E-03	2.0956E-01	3.9683E-02
12-HEPE	0.3558	0.2383	0.1741	0.1754	4.2593E-02	1.7601E-01	2.1301E-01	3.8028E-01
BCAA/Tyr	0.2537	0.4449	0.1248	0.1191	4.3679E-02	2.5295E-04	2.1301E-01	3.4034E-03
20-HETE/AA	-0.3687	0.2193	0.1823	0.1712	4.5018E-02	2.0223E-01	2.1301E-01	4.0175E-01
Met-SO2	-0.3132	-0.2751	0.1552	0.1397	4.5082E-02	5.0705E-02	2.1301E-01	1.4714E-01
LPA (20:5)	0.3288	-0.0327	0.1631	0.1664	4.5337E-02	8.4440E-01	2.1301E-01	9.3612E-01
Arg	-0.3730	-0.7240	0.1874	0.1787	4.8191E-02	7.6624E-05	2.2289E-01	1.7447E-03
TXB1	0.3764	0.1597	0.1915	0.1741	5.0967E-02	3.6053E-01	2.3210E-01	5.5009E-01
8,12-iso-iPF2alpha-VI/AA	-0.3883	-0.1807	0.1983	0.1768	5.1888E-02	3.0832E-01	2.3271E-01	4.9871E-01
PGA2/AA	-0.3478	0.1736	0.1794	0.1544	5.4111E-02	2.6231E-01	2.3906E-01	4.6217E-01
g-Glu-Gln	-0.3893	-0.7733	0.2032	0.1789	5.7068E-02	2.6252E-05	2.4554E-01	7.0641E-04
DHEA	0.2018	0.2400	0.1054	0.1076	5.7282E-02	2.7041E-02	2.4554E-01	9.5287E-02
His	-0.3380	-0.3995	0.1774	0.1662	5.8551E-02	1.7398E-02	2.4554E-01	6.8666E-02
12-KETE	0.3503	0.2351	0.1845	0.1833	5.9311E-02	2.0142E-01	2.4554E-01	4.0175E-01
O-PO3-EA	0.4139	-0.0956	0.2191	0.1869	6.0631E-02	6.0951E-01	2.4554E-01	7.5491E-01
5-HEPE/EPA	-0.2300	-0.2838	0.1219	0.1188	6.0999E-02	1.7982E-02	2.4554E-01	7.0037E-02
LPE (22:6)	-0.3502	-0.5855	0.1859	0.1798	6.1385E-02	1.3550E-03	2.4554E-01	1.1509E-02
Putrescine	0.3474	0.4172	0.1867	0.1796	6.4526E-02	2.1366E-02	2.4840E-01	7.9056E-02
Sum OG	-0.3552	-0.6240	0.1914	0.1759	6.5247E-02	4.9957E-04	2.4840E-01	5.6874E-03
11beta-PGF2alpha/AA	-0.2929	0.1761	0.1577	0.1505	6.5282E-02	2.4399E-01	2.4840E-01	4.4610E-01
AAA	-0.2939	-0.7618	0.1585	0.1537	6.5456E-02	1.6923E-06	2.4840E-01	1.1373E-04
LPS (18:1)	0.3793	-0.0051	0.2053	0.1943	6.6442E-02	9.7896E-01	2.4895E-01	9.9764E-01
OA	-0.3512	-0.4434	0.1907	0.1906	6.7343E-02	2.1197E-02	2.4917E-01	7.9056E-02
TXB2	0.3290	0.0717	0.1807	0.1714	7.0484E-02	6.7634E-01	2.5757E-01	8.2142E-01
Trimethyl-Lys	-0.2811	-0.6666	0.1563	0.1729	7.3912E-02	1.6528E-04	2.6680E-01	2.5809E-03
beta-Ala	-0.3318	-0.1122	0.1855	0.1629	7.5407E-02	4.9205E-01	2.6784E-01	6.6505E-01
Ornithine	-0.3053	-0.5316	0.1722	0.1658	7.8084E-02	1.6065E-03	2.6784E-01	1.2514E-02
LCA	-0.3155	-0.5595	0.1785	0.1718	7.8951E-02	1.3609E-03	2.6784E-01	1.1509E-02
Asn	-0.2359	-0.4002	0.1335	0.1255	7.9082E-02	1.7240E-03	2.6784E-01	1.3084E-02
PGF2alpha/AA	0.3361	0.4576	0.1906	0.1788	7.9683E-02	1.1326E-02	2.6784E-01	4.7894E-02
12-HETE	0.3643	0.0655	0.2067	0.2076	7.9918E-02	7.5266E-01	2.6784E-01	8.6862E-01
LPG (20:3)	0.3310	-0.4886	0.1887	0.1894	8.1295E-02	1.0732E-02	2.6784E-01	4.6037E-02
LPE (14:0)	0.3010	0.0951	0.1717	0.1792	8.1437E-02	5.9608E-01	2.6784E-01	7.4447E-01
Met-SO	-0.3214	-0.4092	0.1843	0.1800	8.3064E-02	2.4217E-02	2.7019E-01	8.7475E-02
PGE1/DGLA	0.3393	0.3336	0.1973	0.1957	8.7391E-02	9.0032E-02	2.8117E-01	2.2174E-01
Saccharopine	-0.3452	-0.6320	0.2031	0.1812	9.1069E-02	6.2105E-04	2.8641E-01	6.8086E-03
5-KETE/5-HETE	0.3022	0.7172	0.1779	0.1804	9.1574E-02	1.0476E-04	2.8641E-01	2.2125E-03
13,14-dihydro-15-keto-PGF2alpha	-0.3128	-0.0047	0.1846	0.1771	9.1922E-02	9.7906E-01	2.8641E-01	9.9764E-01
19,20-DiHDPA	0.3245	-0.0591	0.1928	0.1843	9.4271E-02	7.4891E-01	2.9067E-01	8.6862E-01
LPG (18:3)	0.2401	-0.1557	0.1434	0.1330	9.5954E-02	2.4351E-01	2.9281E-01	4.4610E-01
11,12-EpTrE	-0.2799	-0.2062	0.1688	0.1556	9.9191E-02	1.8679E-01	2.9960E-01	3.9160E-01
5,6-DiHETrE	-0.2730	-0.5583	0.1664	0.1645	1.0268E-01	8.5246E-04	3.0700E-01	8.7010E-03
LPE (18:2)	-0.2825	-0.4407	0.1732	0.1633	1.0464E-01	7.6474E-03	3.0973E-01	3.7109E-02
Met	-0.2962	-0.6022	0.1831	0.1781	1.0763E-01	8.9195E-04	3.1543E-01	8.8006E-03
12-HHTrE	0.2802	0.0673	0.1738	0.1612	1.0881E-01	6.7711E-01	3.1577E-01	8.2142E-01
Gly	-0.2734	-0.3660	0.1728	0.1681	1.1557E-01	3.0853E-02	3.3212E-01	1.0497E-01
LPG (16:1)	0.3089	-0.3667	0.1963	0.1856	1.1748E-01	4.9855E-02	3.3436E-01	1.4634E-01
PGE2/AA	0.2835	0.4952	0.1831	0.1834	1.2365E-01	7.6146E-03	3.4858E-01	3.7109E-02
AABA	0.3000	0.0558	0.1957	0.1902	1.2714E-01	7.6956E-01	3.5033E-01	8.7949E-01
1-Met-His	-0.2907	-0.3472	0.1905	0.1834	1.2879E-01	5.9919E-02	3.5628E-01	1.6124E-01
5-IPF2alpha-VI	0.2876	-0.1511	0.1890	0.1753	1.3003E-01	3.9003E-01	3.5637E-01	5.8014E-01
Sum TxS	0.2877	0.1283	0.1935	0.1815	1.3892E-01	4.8072E-01	3.7725E-01	6.5573E-01
PGE2	0.2868	0.3463	0.1944	0.1931	1.4214E-01	4.7338E-02	3.7927E-01	1.9237E-01
cLPA (18:0)	0.2638	0.0523	0.1789	0.1689	1.4222E-01	7.5711E-01	3.7927E-01	8.6862E-01
15-HETrE	0.2921	0.0636	0.2020	0.1941	1.5005E-01	7.4358E-01	3.9655E-01	8.6862E-01
Sum Pgs	-0.2716	0.3745	0.1887	0.1942	1.5186E-01	5.5414E-02	3.9778E-01	1.5470E-01
11-HETE	0.2842	-0.0079	0.1987	0.1892	1.5458E-01	9.6659E-01	4.0136E-01	9.9764E-01
8,9-DiHETrE	-0.2549	-0.6686	0.1790	0.1691	1.5632E-01	1.1212E-04	4.0234E-01	2.2125E-03
12-HETE/AA	0.2911	0.1894	0.2061	0.2001	1.5975E-01	3.4522E-01	4.0624E-01	5.3499E-01
Arg/Lys	-0.2745	-0.4167	0.1953	0.1849	1.6166E-01	2.5534E-02	4.0624E-01	9.1062E-02
cLPA (20:4)	-0.2434	-0.1244	0.1732	0.1719	1.6195E-01	4.7001E-01	4.0624E-01	6.5011E-01
SDMA	-0.2193	-0.5135	0.1569	0.1558	1.6398E-01	1.1922E-03	4.0789E-01	1.0694E-02

Chapter III

Kyn/Trp	0.2655	0.1725	0.1906	0.1737	1.6547E-01	3.2211E-01	4.0816E-01	5.1219E-01
GCDCA	0.2201	-0.2117	0.1586	0.1451	1.6688E-01	1.4635E-01	4.0823E-01	3.2328E-01
Sum HEPEs	0.2336	0.2636	0.1691	0.1717	1.6894E-01	1.2662E-01	4.0988E-01	2.9055E-01
Sum DiHETrEs	-0.2375	-0.7094	0.1725	0.1626	1.7032E-01	2.2163E-05	4.0988E-01	6.5604E-04
BCAA/AAA	0.1870	0.3682	0.1377	0.1269	1.7619E-01	4.1844E-03	4.1745E-01	2.3369E-02
Lys	-0.2446	-0.6035	0.1801	0.1767	1.7629E-01	7.9425E-04	4.1745E-01	8.3963E-03
LPG (18:1)	0.2627	-0.4876	0.1949	0.1812	1.7937E-01	7.8173E-04	4.2137E-01	3.7321E-02
9-HODE/9-HpODE	0.2328	0.0219	0.1761	0.1844	1.8802E-01	9.0561E-01	4.3823E-01	9.7123E-01
Glu	0.2394	-0.0023	0.1841	0.1909	1.9543E-01	9.9051E-01	4.4828E-01	9.9764E-01
AA	0.2568	-0.2645	0.1981	0.1985	1.9674E-01	1.8442E-01	4.4828E-01	3.9160E-01
5-HETrE/DGLA	-0.2310	-0.3082	0.1782	0.1586	1.9688E-01	5.3605E-02	4.4828E-01	1.5112E-01
Phe	0.2521	-0.1445	0.1967	0.1728	2.0181E-01	4.0439E-01	4.5300E-01	5.9257E-01
LPI (20:4)	0.2209	-0.1108	0.1725	0.1736	2.0201E-01	5.2441E-01	4.5300E-01	6.8381E-01
9-KODE/9-HODE	-0.2248	-0.4730	0.1771	0.1633	2.0597E-01	4.2815E-03	4.5839E-01	2.3469E-02
LPE (20:5)	-0.2351	-0.4242	0.1880	0.1753	2.1266E-01	1.6562E-02	4.6975E-01	6.6249E-02
TXB2/AA	0.2175	0.1731	0.1764	0.1691	2.1940E-01	3.0740E-01	4.8106E-01	4.9871E-01
15-HETE	0.2448	-0.0517	0.2013	0.1989	2.2560E-01	7.9525E-01	4.9101E-01	8.9165E-01
15-HEPE	0.1708	0.1435	0.1469	0.1560	2.4643E-01	3.5924E-01	5.3244E-01	5.5009E-01
DGLA	0.2229	-0.1170	0.1978	0.1903	2.6128E-01	5.3968E-01	5.4721E-01	6.9757E-01
5-OH-Trp	0.2162	-0.4541	0.1922	0.1929	2.6223E-01	1.9711E-02	5.4721E-01	7.5772E-02
cLPA (16:1)	-0.1899	-0.5692	0.1692	0.1800	2.6339E-01	1.8431E-03	5.4721E-01	1.3639E-02
GABA	0.2087	0.3684	0.1861	0.1886	2.6350E-01	5.2357E-02	5.4721E-01	1.4902E-01
ETE	0.2204	-0.3070	0.1967	0.1979	2.6412E-01	1.2264E-01	5.4721E-01	2.8360E-01
8-HETrE	0.2252	0.0659	0.2017	0.1960	2.6573E-01	7.3691E-01	5.4721E-01	8.6862E-01
3-ABA	0.1463	0.0211	0.1312	0.1262	2.6662E-01	8.6751E-01	5.4721E-01	9.4865E-01
SIP (16:1)	-0.1394	-0.4009	0.1255	0.1319	2.6806E-01	2.7479E-03	5.4721E-01	1.6946E-02
9-HEPE	0.1564	0.0825	0.1419	0.1502	2.7198E-01	5.8357E-01	5.5044E-01	7.3819E-01
12-HHTrE/AA	0.1850	0.1488	0.1683	0.1571	2.7338E-01	3.4501E-01	5.5044E-01	5.3499E-01
Pro	0.2056	-0.2374	0.1878	0.1850	2.7522E-01	2.0128E-01	5.5044E-01	4.0175E-01
LPG (22:4)	0.2088	-0.2275	0.1918	0.1799	2.7796E-01	2.0773E-01	5.5220E-01	4.0453E-01
2,3-dinor-8-iso-PGF2alpha	0.2209	-0.0988	0.2082	0.2037	2.9018E-01	6.2815E-01	5.7262E-01	7.7472E-01
Ile	-0.2155	-0.5763	0.2042	0.1959	2.9281E-01	3.7145E-03	5.7398E-01	2.1144E-02
15-HEPE/EPA	-0.1816	0.0603	0.1743	0.1622	2.9903E-01	7.1067E-01	5.8232E-01	8.5511E-01
11,12-DiHETrE	-0.1828	-0.6428	0.1765	0.1541	3.0175E-01	4.7710E-05	5.8287E-01	1.1768E-03
TXB1/DGLA	0.1973	0.1788	0.1910	0.1800	3.0325E-01	3.2178E-01	5.8287E-01	5.1219E-01
LPE (20:3)	-0.1676	-0.6254	0.1645	0.1629	3.0961E-01	1.7326E-04	5.9125E-01	2.5809E-03
LPS (18:2)	0.1667	0.1855	0.1650	0.1639	3.1378E-01	2.5944E-01	5.9538E-01	4.6158E-01
LPA (14:0)	0.1313	-0.0865	0.1338	0.1296	3.2807E-01	5.0537E-01	6.1853E-01	6.6781E-01
LA	0.1379	0.1702	0.1419	0.1364	3.3283E-01	2.1377E-01	6.2179E-01	4.1013E-01
Citrulline	-0.1466	-0.5118	0.1517	0.1531	3.3522E-01	1.0178E-03	6.2179E-01	9.4143E-03
9-HOTrE/ALA	-0.1660	-0.0013	0.1721	0.1677	3.3610E-01	9.9368E-01	6.2179E-01	9.9764E-01
PAF 18(2)	0.1499	0.0906	0.1582	0.1639	3.4479E-01	5.8113E-01	6.3389E-01	7.3819E-01
9-HEPE/EPA	-0.1721	-0.0511	0.1851	0.1779	3.5408E-01	7.7444E-01	6.4696E-01	8.8167E-01
ALA	0.1255	-0.0092	0.1360	0.1272	3.5738E-01	9.4230E-01	6.4899E-01	9.9614E-01
SIP (18:1)	-0.1359	-0.4813	0.1492	0.1533	3.6381E-01	1.9938E-03	6.5639E-01	1.3725E-02
DPA	-0.1692	-0.3166	0.1867	0.1860	3.6589E-01	9.0642E-02	6.5639E-01	2.2174E-01
14-HDoHE/DHA	0.1804	0.2214	0.2002	0.1900	3.6895E-01	2.4566E-01	6.5788E-01	4.4610E-01
12-HEPE/EPA	0.1720	0.2047	0.1979	0.1917	3.8623E-01	2.8706E-01	6.7583E-01	4.8555E-01
Homoserine	-0.1520	-0.6494	0.1752	0.1759	3.8703E-01	2.9918E-04	6.7583E-01	3.8503E-03
delta-17,6-keto-PGF1alpha/EPA	-0.1543	0.3576	0.1779	0.1573	3.8719E-01	2.4233E-02	6.7583E-01	8.7475E-02
11beta-PGF2alpha	-0.1074	-0.0264	0.1242	0.1232	3.8884E-01	8.3086E-01	6.7583E-01	9.2457E-01
5-KETE	0.1861	0.2031	0.2161	0.2013	3.9043E-01	3.1443E-01	6.7583E-01	5.0582E-01
14-HDoHE	0.1705	0.2138	0.2030	0.2092	4.0216E-01	3.0833E-01	6.8982E-01	4.9871E-01
LPG (18:2)	0.1360	-0.1741	0.1622	0.1579	4.0317E-01	2.7199E-01	6.8982E-01	4.7081E-01
5-HEPE	0.1425	-0.1792	0.1733	0.1744	4.1213E-01	3.0545E-01	7.0109E-01	4.9871E-01
PGA2	-0.1539	-0.0556	0.1888	0.1730	4.1601E-01	7.4819E-01	7.0366E-01	8.6862E-01
Citrulline/Omithine	0.1224	-0.0009	0.1543	0.1331	4.2867E-01	9.9445E-01	7.1366E-01	9.9764E-01
Sum HETrEs	0.1546	-0.0166	0.1953	0.1899	4.2994E-01	9.3038E-01	7.1366E-01	9.9420E-01
Sum HETEs	0.1652	-0.2708	0.2088	0.2043	4.3003E-01	1.8683E-01	7.1366E-01	3.9160E-01
19,20-EpDPE	0.1503	0.0086	0.1906	0.1911	4.3157E-01	9.6414E-01	7.1366E-01	9.9764E-01
FA (16:0)	-0.1554	-0.2280	0.1998	0.1952	4.3789E-01	2.4441E-01	7.2009E-01	4.4610E-01
Clupanodonic acid	0.1185	-0.0247	0.1573	0.1533	4.5229E-01	8.7241E-01	7.3698E-01	9.4939E-01
LPA (16:1)	0.1332	-0.1951	0.1771	0.1704	4.5314E-01	2.5367E-01	7.3698E-01	4.5784E-01
9-HODE	0.1321	0.1522	0.1789	0.1800	4.6117E-01	3.9921E-01	7.4594E-01	5.8789E-01
SIP (18:0)	0.1328	-0.2937	0.1815	0.1739	4.6538E-01	9.2976E-02	7.4865E-01	2.2558E-01
8,12-iso-iPF2alpha-VI	-0.1436	-0.4012	0.1979	0.1922	4.6909E-01	3.8375E-02	7.5054E-01	1.1861E-01
Sum DiHETEs	0.1352	-0.0033	0.1897	0.1679	4.726E-01	9.8432E-01	7.5741E-01	9.9764E-01
16-HDoHE	0.1046	0.1029	0.1473	0.1530	4.7850E-01	5.0222E-01	7.5741E-01	6.6781E-01
17-HDoHE/DHA	0.1449	0.1390	0.2056	0.1953	4.8195E-01	4.7768E-01	7.5790E-01	6.5460E-01

Diagnosis of Late-Onset Sepsis

20-HDoHE	0.1261	0.1450	0.1798	0.1776	4.8393E-01	4.1530E-01	7.5790E-01	5.9965E-01
g-Glu-Ala	-0.1292	-0.5192	0.1853	0.1715	4.8664E-01	2.8428E-03	7.5813E-01	1.7173E-02
14,15-DiHETrE	-0.1200	-0.5377	0.1753	0.1664	4.9466E-01	1.4757E-03	7.6273E-01	1.2133E-02
19,20-DiHDPa/19,20-EpDPE	0.1217	-0.0688	0.1781	0.1769	4.9539E-01	6.9785E-01	7.6273E-01	8.4311E-01
11-HETE/AA	0.1343	0.2126	0.1977	0.1928	4.9774E-01	2.7185E-01	7.6273E-01	4.7081E-01
7-HDoHE/DHA	-0.1294	0.1150	0.1931	0.1952	5.0358E-01	5.5662E-01	7.6273E-01	7.1324E-01
16-HDoHE/DHA	0.1259	0.2104	0.1896	0.1945	5.0758E-01	2.8077E-01	7.6273E-01	4.7763E-01
20-HDoHE/DHA	0.1296	0.1853	0.1958	0.1792	5.0876E-01	3.0259E-01	7.6273E-01	4.9871E-01
Sum HODEs	0.1200	0.0823	0.1815	0.1828	5.0954E-01	6.5297E-01	7.6273E-01	7.9868E-01
LPI (22:4)	0.1142	-0.3666	0.1731	0.1716	5.1021E-01	3.4068E-02	7.6273E-01	1.1331E-01
BCAA	-0.1277	-0.5321	0.1965	0.1870	5.1665E-01	4.9778E-03	7.6534E-01	2.6311E-02
Sum SBA	-0.1431	-0.3985	0.2204	0.1895	5.1712E-01	3.6973E-02	7.6534E-01	1.1861E-01
19,20-EpDPE/DHA	0.1047	-0.0240	0.1624	0.1683	5.1991E-01	8.8687E-01	7.6564E-01	9.5606E-01
Coriolic acid	0.1150	0.0062	0.1848	0.1867	5.3473E-01	9.7353E-01	7.7932E-01	9.9764E-01
LPA (22:5)	0.1117	-0.1358	0.1806	0.1821	5.3717E-01	4.5697E-01	7.7932E-01	6.3732E-01
TCA	-0.0949	-0.2182	0.1540	0.1464	5.3878E-01	1.3792E-01	7.7932E-01	3.1163E-01
LPE (18:1)	-0.1054	-0.2184	0.1715	0.1619	5.3974E-01	1.7897E-01	7.7932E-01	3.8389E-01
LPA (20:3)	0.0922	-0.2696	0.1552	0.1564	5.5344E-01	8.6505E-02	7.9108E-01	2.1808E-01
17-HDoHE	0.1012	0.0984	0.1710	0.1745	5.5464E-01	5.7337E-01	7.9108E-01	7.3154E-01
11-HDoHE/DHA	0.1218	0.2807	0.2075	0.1945	5.5805E-01	1.5077E-01	7.9108E-01	3.3057E-01
cLPA (18:2)	-0.0993	-0.1284	0.1694	0.1664	5.5857E-01	4.4121E-01	7.9108E-01	6.1895E-01
FA (18:0)	-0.1084	-0.0314	0.1910	0.1891	5.7095E-01	8.6853E-01	8.0247E-01	9.4865E-01
5-HETE	-0.1115	-0.5929	0.1979	0.1927	5.7409E-01	2.4314E-03	8.0247E-01	1.6357E-02
11-HDoHE	0.1011	0.2008	0.1798	0.1841	5.7478E-01	2.7690E-01	8.0247E-01	4.7378E-01
Ornithine/Arg	0.1104	0.2440	0.1978	0.1967	5.7745E-01	2.1642E-01	8.0247E-01	4.1065E-01
15-HETrE/DGLA	0.1158	0.1871	0.2096	0.1943	5.8126E-01	3.3698E-01	8.0398E-01	5.2775E-01
CA	-0.0999	0.1137	0.1835	0.1703	5.8687E-01	5.0520E-01	8.0797E-01	6.6781E-01
Glutathione	-0.0943	0.1954	0.1755	0.1714	5.9157E-01	2.5611E-01	8.1067E-01	4.5945E-01
5-aminolevulinic acid	-0.0944	-0.0114	0.1844	0.1824	6.0953E-01	9.5034E-01	8.3143E-01	9.9764E-01
2-aminoadipic acid	0.0816	-0.2791	0.1680	0.1537	6.2753E-01	7.1072E-02	8.4552E-01	1.8454E-01
20-HETE	-0.0904	-0.0101	0.1860	0.1894	6.2765E-01	9.5772E-01	8.4552E-01	9.9764E-01
TXB3	0.0879	0.0574	0.1812	0.1702	6.2843E-01	7.3641E-01	8.4552E-01	6.8682E-01
Sum HDoHEs	0.0920	0.1598	0.1916	0.1969	6.3179E-01	4.1814E-01	8.4620E-01	6.0082E-01
O-Acetyl-Ser	-0.0803	-0.1485	0.1738	0.1644	6.4456E-01	3.6788E-01	8.5349E-01	5.5558E-01
Ala	-0.0846	-0.5805	0.1834	0.1845	6.4541E-01	1.9447E-03	8.5349E-01	1.3725E-02
5-HETrE	-0.0857	-0.3280	0.1880	0.1661	6.4914E-01	4.9932E-02	8.5349E-01	1.4634E-01
12,13-EpOME/LA	-0.0821	-0.4994	0.1809	0.1690	6.5048E-01	3.5585E-03	8.5349E-01	2.0653E-02
Arg/ADMA	-0.0923	-0.1877	0.2041	0.1896	6.5165E-01	3.2358E-01	8.5349E-01	5.1219E-01
15-HETE/AA	0.0879	0.1542	0.1971	0.1876	6.5606E-01	4.1204E-01	8.5533E-01	5.9787E-01
TUDCA	0.0791	0.1522	0.1791	0.1685	6.5910E-01	3.6787E-01	8.5533E-01	5.5558E-01
18-HEPE/EPA	0.0801	0.1432	0.1843	0.1777	6.6427E-01	4.2166E-01	8.5533E-01	6.0295E-01
9-HpODE/LA	-0.0840	-0.1924	0.1935	0.1830	6.6462E-01	2.9454E-01	8.5533E-01	4.9536E-01
13-HDoHE	0.0664	0.1794	0.1544	0.1611	6.6778E-01	2.6685E-01	8.5560E-01	4.6738E-01
Cystathionine	-0.0666	-0.2298	0.1584	0.1451	6.7465E-01	1.1528E-01	8.5560E-01	2.7299E-01
LPA (18:0)	0.0703	0.0032	0.1680	0.1653	6.7614E-01	9.8451E-01	8.5560E-01	9.9764E-01
Kyn	-0.0769	-0.4824	0.1864	0.1693	6.8062E-01	4.9123E-03	8.5560E-01	2.6311E-02
Sum LG	-0.0675	-0.2908	0.1638	0.1559	6.8067E-01	6.3893E-02	8.5560E-01	1.6886E-01
LPG (20:4)	0.0661	-0.3063	0.1611	0.1601	6.8217E-01	5.7358E-02	8.5560E-01	1.5867E-01
HomoCys	-0.0760	-0.2860	0.1945	0.1908	6.9627E-01	1.3580E-01	8.6693E-01	3.0920E-01
LPA (18:1)	0.0683	-0.1869	0.1753	0.1711	6.9705E-01	2.7627E-01	8.6693E-01	4.7378E-01
w3FA/w6FA	-0.0410	0.2216	0.1097	0.1090	7.0895E-01	4.3580E-02	8.7464E-01	1.3030E-01
Homocitrulline	-0.0609	-0.4144	0.1633	0.1562	7.0979E-01	8.7174E-03	8.7464E-01	3.9683E-02
Leu	-0.0754	-0.4984	0.2047	0.1963	7.1298E-01	1.2031E-02	8.7464E-01	4.9736E-02
12,13-DiHOME	0.0492	-0.0714	0.1345	0.1312	7.1508E-01	5.8720E-01	8.7464E-01	7.3962E-01
Cys/Cystathionine	0.0688	0.0076	0.2015	0.1860	7.3309E-01	9.6749E-01	8.8548E-01	9.9764E-01
Sum AG	0.0626	-0.3421	0.1839	0.1637	7.3374E-01	3.8104E-02	8.8548E-01	1.1861E-01
3-Met-His	-0.0642	0.0496	0.1886	0.1824	7.3391E-01	7.8592E-01	8.8548E-01	8.8588E-01
12,13-DiHOME/12,13-EpOME	0.0445	0.1584	0.1316	0.1242	7.3591E-01	2.0389E-01	8.8548E-01	4.0234E-01
13-HDoHE/DHA	0.0635	0.3031	0.1926	0.1949	7.4210E-01	1.2163E-01	8.8932E-01	2.8349E-01
LPE (16:1)	-0.0589	-0.3228	0.1817	0.1719	7.4608E-01	6.2401E-02	8.9019E-01	1.6640E-01
9-HOTrE	-0.0540	-0.0128	0.1704	0.1726	7.5148E-01	9.4102E-01	8.9019E-01	9.9614E-01
TXB3/EPA	-0.0532	-0.0753	0.1681	0.1627	7.5185E-01	6.4413E-01	8.9019E-01	7.9113E-01
GCA	0.0629	-0.4109	0.2051	0.1858	7.5952E-01	2.8346E-02	8.9568E-01	9.8709E-02
HCA	-0.0546	0.2175	0.1872	0.1662	7.7089E-01	1.9235E-01	9.0322E-01	3.9765E-01
Val	-0.0535	-0.4558	0.1843	0.1739	7.7201E-01	9.5438E-03	9.0322E-01	4.2164E-02
8-HDoHE/DHA	-0.0495	0.2465	0.1785	0.1980	7.8176E-01	2.1476E-01	9.0649E-01	4.1013E-01
7-HDoHE	-0.0416	0.0493	0.1525	0.1582	7.8538E-01	7.5583E-01	9.0649E-01	8.6862E-01

Chapter III

Mead.Acid	-0.0504	-0.3476	0.1849	0.1828	7.8543E-01	5.8928E-02	9.0649E-01	1.6124E-01
12-KETE/12-HETE	0.0536	0.4038	0.1982	0.1833	7.8705E-01	2.8908E-02	9.0649E-01	9.9498E-02
10-HDoHE/DHA	0.0540	0.0613	0.2046	0.1896	7.9205E-01	7.4704E-01	9.0871E-01	8.6862E-01
Sarcosine	-0.0460	-0.3093	0.1839	0.1812	8.0265E-01	8.9640E-02	9.1205E-01	2.2174E-01
10-HDoHE	0.0459	0.0618	0.1842	0.1896	8.0368E-01	7.4485E-01	9.1205E-01	8.6862E-01
AEA	0.0331	0.1547	0.1332	0.1487	8.0420E-01	2.9973E-01	9.1205E-01	4.9842E-01
Cys	0.0382	-0.1976	0.1716	0.1750	8.2416E-01	2.6042E-01	9.2337E-01	4.6158E-01
2,3-dinor-8-iso-PGF2alpha/AA	0.0442	0.1351	0.2029	0.2019	8.2801E-01	5.0430E-01	9.2337E-01	6.6781E-01
Sum BA	0.0463	0.2568	0.2143	0.2006	8.2917E-01	2.0214E-01	9.2337E-01	4.0175E-01
8-HETrE/DGLA	0.0438	0.1663	0.2033	0.1871	8.2980E-01	3.7533E-01	9.2337E-01	5.6395E-01
3-Methoxytyramine	0.0436	0.2855	0.2044	0.2002	8.3138E-01	1.5591E-01	9.2337E-01	3.3933E-01
5-iPF2alpha-VI/AA	0.0400	0.0519	0.1894	0.1863	8.3290E-01	7.8097E-01	9.2337E-01	8.8570E-01
GLA	-0.0390	-0.5070	0.1918	0.1668	8.3910E-01	2.7402E-03	9.2677E-01	1.6946E-02
DHA	0.0299	-0.0004	0.1509	0.1496	8.4319E-01	9.9764E-01	9.2782E-01	9.9764E-01
9-KODE	0.0351	-0.1256	0.1854	0.1754	8.5004E-01	4.7495E-01	9.3189E-01	6.5388E-01
Glu/GABA	-0.0250	-0.3940	0.1720	0.1692	8.8451E-01	2.1053E-02	9.6531E-01	7.9056E-02
LPA (22:6)	-0.0247	-0.2869	0.1738	0.1803	8.8704E-01	1.1342E-01	9.6531E-01	2.7074E-01
Sum PBA	0.0268	0.1897	0.1991	0.1942	8.9295E-01	3.2981E-01	9.6818E-01	5.1927E-01
LPA (16:0)	0.0198	-0.1129	0.1562	0.1520	8.9935E-01	4.5861E-01	9.6906E-01	6.3732E-01
AA	0.0234	-0.3612	0.1869	0.1904	9.0031E-01	5.9525E-02	9.6906E-01	1.6124E-01
Sum iPs	0.0191	0.0256	0.1730	0.1750	9.1241E-01	8.8369E-01	9.7661E-01	9.5606E-01
LPA (18:2)	-0.0160	-0.1886	0.1537	0.1548	9.1709E-01	2.2465E-01	9.7661E-01	4.2355E-01
8-HDoHE	0.0150	0.1072	0.1480	0.1571	9.1957E-01	4.9571E-01	9.7661E-01	6.6696E-01
17,18-DiHETE	0.0176	-0.0040	0.1859	0.1702	9.2473E-01	9.8109E-01	9.7661E-01	9.9764E-01
TLCA-3S	0.0188	-0.5066	0.2024	0.1868	9.2596E-01	7.3618E-03	9.7661E-01	3.7109E-02
LPE (22:5)	0.0178	-0.2210	0.1954	0.1831	9.2754E-01	2.2906E-01	9.7661E-01	4.2913E-01
Cystathionine/Ho moCys	0.0169	0.0476	0.1929	0.1760	9.3042E-01	7.8712E-01	9.7661E-01	8.8588E-01
11,12-DiHETrE/11,12-EpETrE	-0.0113	-0.4318	0.1683	0.1539	9.4660E-01	5.6041E-03	9.8669E-01	2.9102E-02
cLPA (14:0)	0.0087	-0.2732	0.1338	0.1285	9.4823E-01	3.4901E-02	9.8669E-01	1.1479E-01
PAF (16:0)	0.0127	-0.3356	0.2025	0.1949	9.5002E-01	8.6936E-02	9.8669E-01	2.1808E-01
THDCA	0.0060	0.1080	0.1324	0.1271	9.6419E-01	3.9654E-01	9.9016E-01	5.8688E-01
LPE (18:3)	-0.0072	-0.1267	0.1634	0.1592	9.6514E-01	4.2722E-01	9.9016E-01	6.0797E-01
LPA (20:4)	0.0072	-0.3551	0.1647	0.1694	9.6531E-01	3.7517E-02	9.9016E-01	1.1861E-01
EA	0.0058	0.1977	0.1554	0.1515	9.7023E-01	1.9376E-01	9.9016E-01	3.9765E-01
9-HpODE	-0.0059	-0.0233	0.1738	0.1653	9.7274E-01	8.8823E-01	9.9016E-01	9.5606E-01
LPA (22:4)	-0.0063	-0.4215	0.2054	0.2021	9.7539E-01	3.8469E-02	9.9016E-01	1.1861E-01
cLPA (18:1)	-0.0044	-0.1533	0.1698	0.1667	9.7948E-01	3.5926E-01	9.9016E-01	5.5009E-01
Tau	-0.0043	0.2280	0.1728	0.1793	9.8013E-01	2.0526E-01	9.9016E-01	4.0237E-01
LPS (20:4)	-0.0021	-0.2288	0.1509	0.1437	9.8905E-01	1.1320E-01	9.9521E-01	2.7074E-01
delta-17,6-keto-PGF1alpha	-0.0020	0.3685	0.1987	0.1762	9.9186E-01	3.7954E-02	9.9521E-01	1.1861E-01
12,13-EpOME	0.0011	-0.3358	0.1901	0.1813	9.9521E-01	6.5621E-02	9.9521E-01	1.7189E-01

Table S9: Linear mixed-effect model results of the gender-stratified "Sepsis" models

Metabolite	Estimate Male	Estimate Female	Standard Error Male	Standard Error Female	p-value Male	p-value Female	Adjusted p-value Male	Adjusted p-value Female
LPS (18:0)	0.9835	0.6412	0.1792	0.2079	2.3966E-07	2.7957E-03	7.0939E-05	4.3555E-02
5-HT/Trp	0.9804	0.5125	0.1999	0.2085	2.8845E-06	1.6268E-02	4.2691E-04	1.2038E-01
Thr	-0.7648	-0.7188	0.1656	0.1764	9.5092E-06	1.2955E-04	9.3824E-04	7.6691E-03
Sum DiHETrEs	-0.6859	-0.0517	0.1535	0.2219	1.7806E-05	8.1627E-01	1.3176E-03	8.9888E-01
4-OH-Pro/Pro	-0.7529	-0.6721	0.1748	0.1993	3.3213E-05	1.1506E-03	1.5377E-03	2.6199E-02
LPI (18:0)	0.7168	0.8092	0.1664	0.2266	3.3626E-05	6.0786E-04	1.5377E-03	1.9992E-02
Phe/Tyr	0.5168	0.6575	0.1206	0.1431	3.6364E-05	1.6007E-05	1.5377E-03	4.4175E-03
g-Glu-Gln	-0.7135	-0.4728	0.1684	0.2726	4.4527E-05	6.6875E-02	1.5949E-03	2.8838E-01
Cortisol	0.7922	0.4865	0.1882	0.1957	4.9702E-05	1.5136E-02	1.5949E-03	1.1788E-01
LPE (16:0)	0.6815	0.4827	0.1629	0.1910	5.3881E-05	1.3468E-02	1.5949E-03	1.1074E-01
5-HT	0.8156	0.2327	0.1989	0.2190	7.4247E-05	2.9142E-01	1.9979E-03	5.8201E-01
8,9-DiHETrE	-0.6666	-0.0049	0.1679	0.2249	1.2300E-04	9.8258E-01	3.0132E-03	9.8926E-01
OH-Lys	-0.6935	-0.7813	0.1757	0.1919	1.3234E-04	1.1441E-04	3.0132E-03	7.6691E-03
4-OH-Pro	-0.6836	-0.8182	0.1760	0.1899	1.6657E-04	4.7330E-05	3.5218E-03	4.6699E-03
Sum OG	-0.6989	-0.2531	0.1835	0.2536	2.1764E-04	3.2132E-01	4.2947E-03	5.9628E-01
Trimethyl-Lys	-0.5500	-0.2593	0.1464	0.2468	2.7547E-04	2.9672E-01	5.0963E-03	5.8201E-01
AAA	-0.5199	-0.7609	0.1408	0.2146	3.3234E-04	7.2826E-04	5.3369E-03	2.1556E-02
LPI (16:0)	0.6261	0.9305	0.1698	0.2391	3.3652E-04	2.1483E-04	5.3369E-03	1.0598E-02
Tyr	-0.4946	-0.6681	0.1351	0.1818	3.7156E-04	4.4797E-04	5.3369E-03	1.6575E-02

Diagnosis of Late-Onset Sepsis

11,12-DiHETrE	-0.5577	-0.1642	0.1524	0.2326	3.7235E-04	4.8215E-01	5.3369E-03	7.0652E-01
Saccharopine	-0.6625	-0.3651	0.1813	0.2607	3.7863E-04	1.6534E-01	5.3369E-03	4.2931E-01
Gly-Pro	-0.5781	-0.3344	0.1617	0.1935	4.9710E-04	8.8658E-02	6.6883E-03	2.8838E-01
Trp	-0.5061	-0.8006	0.1484	0.1787	8.7954E-04	2.9848E-05	1.1319E-02	4.4175E-03
5,6-DiHETrE	-0.5267	-0.0444	0.1558	0.2139	9.7050E-04	8.3631E-01	1.969E-02	9.1010E-01
BCAA/Tyr	0.4106	0.4245	0.1231	0.1448	1.1187E-03	4.3923E-03	1.3245E-02	6.1910E-02
delta-17,6-keto-PGF1alpha	0.5150	-0.2750	0.1564	0.2798	1.2897E-03	3.2871E-01	1.3811E-02	5.9939E-01
3-Methoxy-tyrosine	-0.5659	-0.6842	0.1718	0.2124	1.2936E-03	1.8715E-03	1.3811E-02	3.6930E-02
Gln	-0.5335	-0.7040	0.1624	0.2626	1.3247E-03	8.9801E-03	1.3811E-02	9.1002E-02
PGF2alpha/AA	0.5990	0.2702	0.1827	0.2516	1.3531E-03	2.8612E-01	1.3811E-02	5.8201E-01
14,15-DiHETrE	-0.4923	-0.0693	0.1518	0.2471	1.5132E-03	7.7981E-01	1.4930E-02	8.9001E-01
PGF2alpha	0.6096	0.2698	0.1898	0.2677	1.6760E-03	3.1656E-01	1.6003E-02	5.9305E-01
5-KETE/5-HETE	0.6045	0.2131	0.1939	0.1896	2.3037E-03	2.6519E-01	2.0688E-02	5.6473E-01
ADMA	-0.5545	-0.7599	0.1784	0.2206	2.3340E-03	9.4361E-04	2.0688E-02	2.3276E-02
Gly-Gly	0.4745	-0.1517	0.1522	0.2258	2.3764E-03	5.0395E-01	2.0688E-02	7.1120E-01
Arg	-0.5809	-0.7448	0.1918	0.2138	2.9883E-03	8.0436E-04	2.5128E-02	2.1645E-02
5-HETE/AA	-0.4912	0.0160	0.1626	0.2281	3.0562E-03	9.4428E-01	2.5128E-02	9.6715E-01
Sphinganine18.0	0.5505	0.4595	0.1837	0.2553	3.3010E-03	7.6050E-02	2.6408E-02	2.6799E-01
LCA	-0.5239	-0.2322	0.1782	0.2370	3.9494E-03	3.3016E-01	2.9934E-02	5.9939E-01
PGE2/AA	0.5739	0.2140	0.1956	0.2342	3.9788E-03	3.6388E-01	2.9934E-02	6.1901E-01
BCAA/AAA	0.3639	0.3535	0.1242	0.1717	4.0451E-03	4.2761E-02	2.9934E-02	2.0091E-01
LPE (22:6)	-0.5126	-0.4498	0.1823	0.2154	5.7300E-03	4.0141E-02	4.1331E-02	1.9478E-01
delta-17,6-keto-PGF1alpha/EPA	0.4147	-0.3962	0.1478	0.2421	5.8645E-03	1.0632E-01	4.1331E-02	3.1789E-01
5-HETE	-0.5162	0.1024	0.1866	0.2528	6.5197E-03	6.8652E-01	4.4880E-02	8.3190E-01
OH-Lys/Lys	-0.4331	-0.1976	0.1603	0.2386	7.8975E-03	4.1009E-01	5.3129E-02	6.6696E-01
Homoserine	-0.4616	-0.3302	0.1735	0.2357	8.8174E-03	1.6530E-01	5.7669E-02	4.2931E-01
LPE (18:2)	-0.4409	-0.1894	0.1660	0.1983	8.9621E-03	3.4222E-01	5.7669E-02	5.9939E-01
Gln/Glu	-0.4520	-0.5874	0.1708	0.2859	9.1749E-03	4.3891E-02	5.7782E-02	2.0300E-01
g-Glu-Ala	-0.4835	-0.0981	0.1850	0.2071	1.0058E-02	6.3717E-01	6.2023E-02	7.9967E-01
S1P (18:2)	-0.3718	-0.5727	0.1450	0.1963	1.1509E-02	4.6338E-03	6.9042E-02	6.2346E-02
PGE1/DGLA	0.4889	0.2342	0.1910	0.2418	1.1663E-02	3.3623E-01	6.9042E-02	5.9939E-01
Arg/Lys	-0.4838	-0.4211	0.1929	0.2433	1.3549E-02	8.7423E-02	7.7478E-02	2.8838E-01
PGE1	0.4582	0.5220	0.1836	0.2714	1.3878E-02	5.8416E-02	7.7478E-02	2.3612E-01
LPS (16:0)	0.4597	0.3755	0.1844	0.2388	1.4002E-02	1.2002E-01	7.7478E-02	3.5095E-01
LPE (18:0)	0.3940	0.5039	0.1583	0.1714	1.4134E-02	4.3279E-03	7.7478E-02	6.1910E-02
12,13-EpOME/LA	-0.4044	-0.4122	0.1650	0.2251	1.5636E-02	7.1034E-02	8.4018E-02	2.6573E-01
Lys	-0.3775	-0.5646	0.1543	0.2261	1.5895E-02	1.5163E-02	8.4018E-02	1.1788E-01
GABA	0.4497	0.1749	0.1848	0.2604	1.6402E-02	5.0372E-01	8.5174E-02	7.1120E-01
11,12-DiHETrE/11,12-EpETrE	-0.3710	-0.0649	0.1539	0.2408	1.7351E-02	7.8829E-01	8.8551E-02	8.9058E-01
Sphingosine18.1	0.4505	0.4055	0.1887	0.2402	1.8448E-02	9.6007E-02	9.2551E-02	3.0557E-01
LPE (20:4)	-0.3878	-0.6112	0.1647	0.1865	2.0110E-02	1.5547E-03	9.9209E-02	3.2872E-02
LPE (22:4)	-0.3785	-0.4270	0.1620	0.1685	2.1057E-02	1.3244E-02	1.0218E-01	1.1074E-01
Met	-0.3943	-0.5441	0.1733	0.2030	2.4706E-02	9.5467E-03	1.1642E-01	9.1002E-02
PGE2	0.4690	0.2462	0.2064	0.2441	2.4779E-02	3.1642E-01	1.1642E-01	5.9305E-01
PAF 16(0)	-0.4444	0.3424	0.1968	0.2396	2.5679E-02	1.5677E-01	1.1809E-01	4.2186E-01
LPS (22:4)	0.3949	0.6828	0.1752	0.2510	2.6186E-02	8.0015E-03	1.1809E-01	9.1002E-02
Sum PGs	0.4433	-0.3531	0.1972	0.2591	2.6330E-02	1.7685E-01	1.1809E-01	4.3988E-01
Asp	0.3967	-0.1062	0.1792	0.2599	2.8988E-02	6.8387E-01	1.2807E-01	8.3190E-01
Asn	-0.3546	-0.4458	0.1610	0.1423	2.9623E-02	2.4310E-03	1.2895E-01	4.1607E-02
1-Met-His	-0.3714	-0.3126	0.1721	0.2430	3.2857E-02	2.0199E-01	1.4095E-01	4.6709E-01
SDMA	-0.3082	-0.4705	0.1466	0.2225	3.7487E-02	3.7606E-02	1.5654E-01	1.8968E-01
LPE (20:3)	-0.3554	-0.5009	0.1693	0.1788	3.7818E-02	6.3889E-03	1.5654E-01	7.5644E-02
LPE (20:5)	-0.3654	-0.1972	0.1743	0.2191	3.8078E-02	3.7097E-01	1.5654E-01	6.2747E-01
LPS (22:6)	0.3055	0.2239	0.1480	0.1542	4.1145E-02	1.5051E-01	1.6446E-01	4.0872E-01
Glu/GABA	-0.3560	0.0007	0.1726	0.2327	4.1248E-02	9.9766E-01	1.6446E-01	9.9821E-01
GLA	-0.4033	-0.0203	0.1960	0.2113	4.1671E-02	9.2379E-01	1.6446E-01	9.6536E-01
TXB2/AA	0.3346	0.0228	0.1635	0.2271	4.3012E-02	2.0333E-01	1.6752E-01	9.6536E-01
Putrescine	0.3560	0.5279	0.1766	0.2224	4.5976E-02	2.0214E-02	1.7580E-01	1.3296E-01
12-HHTrE/AA	0.3046	-0.0734	0.1512	0.2218	4.6327E-02	7.4148E-01	1.7580E-01	8.6821E-01
5-HEPE/EPA	-0.2514	-0.1735	0.1263	0.1492	4.8735E-02	2.4834E-01	1.8135E-01	5.4450E-01
cLPA (16:1)	-0.3420	-0.5597	0.1724	0.2116	4.9500E-02	9.8381E-03	1.8135E-01	9.1002E-02
Sum TXs	0.3230	0.0829	0.1628	0.2569	4.9625E-02	7.4795E-01	1.8135E-01	8.6979E-01
Sum LG	-0.3053	0.1392	0.1575	0.2102	5.4808E-02	5.0960E-01	1.9784E-01	7.1151E-01
8,12-iso-iPF2alpha-VI	-0.3289	0.0757	0.1702	0.2546	5.5534E-02	7.6709E-01	1.9794E-01	8.8350E-01
Ornithine	-0.3351	-0.4157	0.1739	0.2222	5.6171E-02	6.5324E-02	1.9794E-01	2.5442E-01
TLCA-3S	-0.3570	-0.2139	0.1890	0.2472	6.1281E-02	3.8955E-01	2.1340E-01	6.4779E-01
12-HHTrE	0.2858	0.0274	0.1522	0.2330	6.2773E-02	9.0666E-01	2.1606E-01	9.6190E-01
LPI (16:1)	0.3225	0.0595	0.1759	0.2179	6.9185E-02	7.8550E-01	2.3508E-01	8.9058E-01

Chapter III

TXB2	0.2975	0.1696	0.1628	0.2330	7.0182E-02	4.6888E-01	2.3508E-01	7.0243E-01
Homocitrulline	-0.2934	-0.2058	0.1609	0.2074	7.0683E-02	3.2433E-01	2.3508E-01	5.9628E-01
5-HETrE/DGLA	-0.3019	-0.2188	0.1703	0.2156	7.8773E-02	3.1331E-01	2.5908E-01	5.9305E-01
LPI (18:1)	0.3151	0.5814	0.1787	0.2213	8.0751E-02	1.0357E-02	2.6122E-01	9.2901E-02
Citrulline	-0.2991	-0.6508	0.1701	0.1736	8.1189E-02	3.3441E-04	2.6122E-01	1.4141E-02
Gly	-0.2971	-0.3172	0.1718	0.2030	8.6186E-02	1.2273E-01	2.7431E-01	3.5113E-01
S-Methyl-Cys	-0.2753	-0.4787	0.1631	0.2422	9.3976E-02	5.5919E-02	2.9207E-01	2.2259E-01
12-HETE/AA	0.3225	0.2828	0.1918	0.2611	9.5147E-02	2.8215E-01	2.9207E-01	5.8201E-01
Ser	-0.3158	-0.5197	0.1880	0.2214	9.5491E-02	2.2069E-02	2.9207E-01	1.3625E-01
LPE (14:0)	0.3006	-0.1121	0.1791	0.2087	9.5711E-02	5.9270E-01	2.9207E-01	7.6631E-01
Met-SO2	-0.2517	-0.2781	0.1522	0.1785	1.0095E-01	1.2337E-01	3.0002E-01	3.5113E-01
Sum AG	-0.2913	0.1281	0.1765	0.2290	1.0132E-01	5.7746E-01	3.0002E-01	7.6307E-01
11,12-EpETrE	-0.2700	0.0641	0.1639	0.1941	1.0199E-01	7.4209E-01	3.0002E-01	8.6821E-01
Met-SO	-0.2993	-0.2569	0.1820	0.2218	1.0264E-01	2.5087E-01	3.0002E-01	5.4600E-01
TXB1	0.2710	0.2094	0.1652	0.2506	1.0338E-01	4.0605E-01	3.0002E-01	6.6404E-01
9-HpODE/LA	-0.2767	-0.0669	0.1700	0.2405	1.0619E-01	7.8177E-01	3.0237E-01	8.9001E-01
beta-Ala	-0.2853	-0.1656	0.1758	0.2126	1.0712E-01	4.3847E-01	3.0237E-01	6.7598E-01
Sum SBA	-0.3101	-0.0111	0.1911	0.2833	1.0726E-01	9.6878E-01	3.0237E-01	9.8130E-01
5-HETrE	-0.2757	-0.1208	0.1716	0.2272	1.1069E-01	5.9635E-01	3.0909E-01	7.6631E-01
OA	-0.3228	-0.2885	0.2041	0.2370	1.1632E-01	2.2716E-01	3.2178E-01	5.1328E-01
Sum KETEs	0.3002	0.6376	0.1922	0.2236	1.2094E-01	5.5696E-03	3.2733E-01	6.8692E-02
12,13-EpOME	-0.2903	-0.0905	0.1862	0.2295	1.2144E-01	6.9419E-01	3.2733E-01	8.3190E-01
9-KODE/9-HODE	-0.2746	-0.3708	0.1762	0.2102	1.2164E-01	8.1592E-02	3.2733E-01	2.8083E-01
LPG (18:1)	-0.2915	0.2095	0.1882	0.2263	1.2398E-01	3.5749E-01	3.3062E-01	6.1167E-01
LPS (18:2)	0.2625	0.2959	0.1723	0.2141	1.3041E-01	1.7071E-01	3.4465E-01	4.3187E-01
DPA	-0.2744	-0.1883	0.1808	0.2334	1.3165E-01	4.2219E-01	3.4485E-01	6.7152E-01
DEA	0.2539	0.5330	0.1723	0.2729	1.4320E-01	5.4862E-02	3.7182E-01	2.3008E-01
HCA	0.2447	-0.0777	0.1673	0.2301	1.4613E-01	7.3648E-01	3.7612E-01	6.821E-01
Glutathione	0.1878	0.0555	0.1312	0.2828	1.5480E-01	8.4480E-01	3.9057E-01	9.1322E-01
Kyn/Trp	0.2382	0.4110	0.1666	0.2693	1.5566E-01	1.3094E-01	3.9057E-01	3.6564E-01
LPG (20:4)	-0.2117	-0.0127	0.1482	0.1944	1.5570E-01	9.4823E-01	3.9057E-01	9.6785E-01
Mead.Acid	-0.2402	-0.2081	0.1691	0.2487	1.5784E-01	4.0544E-01	3.9259E-01	6.6404E-01
S1P (16:1)	-0.1898	-0.3650	0.1340	0.1741	1.5916E-01	3.9234E-02	3.9259E-01	1.9356E-01
PGF1alpha	0.1790	-0.4441	0.1279	0.1905	1.6416E-01	2.2309E-02	4.0158E-01	1.3625E-01
8-iso-PGF3alpha	-0.1481	-0.1159	0.1073	0.1978	1.7053E-01	5.5970E-01	4.1375E-01	7.5649E-01
11,12-EpETrE/AA	-0.2495	-0.0519	0.1824	0.2213	1.7374E-01	8.1520E-01	4.1812E-01	8.9888E-01
LPE (18:1)	-0.2341	-0.0740	0.1726	0.1778	1.7742E-01	6.7840E-01	4.2351E-01	8.3190E-01
11-HETE/AA	0.2557	0.0837	0.1905	0.2637	1.8196E-01	7.5163E-01	4.3087E-01	8.6979E-01
19,20-EpDPE/DHA	-0.2130	0.4491	0.1602	0.2423	1.8615E-01	6.7583E-02	4.3472E-01	2.5980E-01
Ile	-0.2530	-0.5583	0.1910	0.2312	1.8788E-01	1.912E-02	4.3472E-01	1.3225E-01
5-HEPE	-0.2186	0.3951	0.1655	0.2403	1.8884E-01	1.0406E-01	4.3472E-01	3.1703E-01
TCA	-0.2161	0.1469	0.1638	0.1809	1.8945E-01	4.1956E-01	4.3472E-01	6.7152E-01
12-HEPE	0.2352	0.5179	0.1792	0.2094	1.9173E-01	1.5531E-02	4.3656E-01	1.1788E-01
AABA	0.2463	-0.1342	0.1888	0.2536	1.9439E-01	5.9803E-01	4.3924E-01	7.6631E-01
GCA	-0.2226	-0.1551	0.1749	0.2763	2.0554E-01	5.7624E-01	4.5878E-01	7.6307E-01
12-HEPE/EPA	0.2364	0.2334	0.1860	0.2464	2.0614E-01	3.4648E-01	4.5878E-01	5.9975E-01
15-HETE/AA	0.2417	0.1635	0.1920	0.2463	2.1034E-01	5.0880E-01	4.5916E-01	7.1151E-01
3-Methoxytyramine	0.2739	0.1043	0.2178	0.2631	2.1089E-01	6.9290E-01	4.5916E-01	8.3190E-01
12-HETE	0.2496	0.3071	0.1985	0.2599	2.1096E-01	2.4096E-01	4.5916E-01	5.3227E-01
TXB1/DGLA	0.2256	0.0565	0.1803	0.2419	2.1326E-01	8.1581E-01	4.6078E-01	8.9888E-01
19,20-EpDPE	-0.2155	0.5892	0.1746	0.2611	2.1947E-01	2.6783E-02	4.7074E-01	1.5545E-01
LPA (22:4)	-0.2310	-0.1052	0.1883	0.2660	2.2227E-01	6.9390E-01	4.7333E-01	8.3190E-01
3-AIBA	0.1362	-0.1569	0.1143	0.1540	2.3573E-01	3.1247E-01	4.9583E-01	5.9305E-01
8,12-iso-iPF2alpha-VI/AA	-0.2285	-0.1104	0.1919	0.2289	2.3619E-01	6.3110E-01	4.9583E-01	7.9831E-01
Tau	0.1994	0.0005	0.1714	0.2131	2.4690E-01	9.9821E-01	5.1466E-01	9.9821E-01
Kyn	-0.1923	-0.3320	0.1661	0.2689	2.4919E-01	2.2074E-01	5.1545E-01	5.0385E-01
LPA (22:6)	-0.2087	0.0512	0.1816	0.2017	2.5254E-01	8.0052E-01	5.1545E-01	8.9755E-01
LPI (14:0)	0.1744	0.0860	0.1522	0.1947	2.5423E-01	6.5989E-01	5.1545E-01	8.2070E-01
Arg/ADMA	-0.2309	-0.2587	0.2020	0.2474	2.5512E-01	2.9887E-01	5.1545E-01	5.8201E-01
9-HpODE	-0.1762	0.1582	0.1544	0.2179	2.5598E-01	4.6987E-01	5.1545E-01	7.0243E-01
AdA	-0.2050	-0.0546	0.1805	0.2428	2.5837E-01	8.2277E-01	5.1674E-01	8.9888E-01
BCAA	-0.2025	-0.5093	0.1814	0.2255	2.6654E-01	2.7915E-02	5.2643E-01	1.5890E-01
LPE (18:3)	-0.1788	0.0178	0.1603	0.2016	2.6677E-01	9.2973E-01	5.2643E-01	9.6536E-01
Ornithine/Arg	0.2146	0.4279	0.1998	0.2603	2.8520E-01	1.0418E-01	5.5906E-01	3.1703E-01
DHEA	0.1127	0.4310	0.1078	0.1366	2.9795E-01	2.2543E-03	5.7870E-01	4.1607E-02
Sum PBA	0.1883	0.2161	0.1806	0.2625	2.9913E-01	4.1281E-01	5.7870E-01	6.6772E-01
His	-0.1542	-0.7114	0.1527	0.2470	3.1438E-01	5.2078E-03	6.0407E-01	6.7022E-02
LPG (18:2)	-0.1682	0.1146	0.1672	0.1795	3.1632E-01	5.2522E-01	6.0407E-01	7.2648E-01
Phe	0.1605	-0.0779	0.1613	0.2778	3.2169E-01	7.7997E-01	6.0657E-01	8.9001E-01
Ala	-0.1747	-0.4887	0.1756	0.2422	3.2173E-01	4.7244E-02	6.0657E-01	2.1188E-01
Cystathionine	-0.1320	-0.0859	0.1342	0.2044	3.2741E-01	6.7547E-01	6.1203E-01	8.3190E-01

Diagnosis of Late-Onset Sepsis

2,3-dinor-8-iso-PGF2alpha/AA	0.1883	-0.2376	0.1921	0.2505	3.2876E-01	3.4601E-01	6.1203E-01	5.9975E-01
LPG (14:0)	0.1141	-0.0935	0.1191	0.1613	3.3962E-01	5.6371E-01	6.2587E-01	7.5844E-01
TUDCA	0.1674	0.3504	0.1749	0.2483	3.4042E-01	1.6236E-01	6.2587E-01	4.2909E-01
SIP (18:1)	-0.1437	-0.4979	0.1535	0.2109	3.5090E-01	2.0872E-02	6.3623E-01	1.3431E-01
9-HODE/9-HpODE	0.1821	0.2275	0.1966	0.2137	3.5610E-01	2.9032E-01	6.3623E-01	5.8201E-01
LPA (18:2)	-0.1449	0.2037	0.1565	0.1798	3.5612E-01	2.6179E-01	6.3623E-01	5.6153E-01
LPI (22:4)	-0.1481	-0.0957	0.1602	0.2378	3.5697E-01	6.8828E-01	6.3623E-01	8.3190E-01
LPA (20:3)	-0.1351	0.0863	0.1467	0.2152	3.5893E-01	6.8935E-01	6.3623E-01	8.3190E-01
12,13-DiHOME/12,13-EpOME	0.1160	0.1592	0.1260	0.1508	3.5896E-01	2.9463E-01	6.3623E-01	5.8201E-01
FA (16:0)	-0.1788	-0.1871	0.1964	0.2523	3.6426E-01	4.6056E-01	6.3785E-01	6.9554E-01
CA	0.1550	-0.1533	0.1707	0.2426	3.6563E-01	5.2938E-01	6.3785E-01	7.2882E-01
9-HOTe/ALA	-0.1507	0.0807	0.1668	0.2172	3.6793E-01	7.1144E-01	6.3785E-01	8.4914E-01
Val	-0.1520	-0.4275	0.1697	0.2154	3.7217E-01	5.1888E-02	6.3785E-01	2.2259E-01
cLPA (18:0)	0.1497	0.2416	0.1689	0.2307	3.7694E-01	2.9812E-01	6.3785E-01	5.8201E-01
LPG (20:3)	-0.1694	0.1796	0.1912	0.2035	3.7718E-01	3.8023E-01	6.3785E-01	6.3948E-01
12-KETE	0.1671	0.5371	0.1889	0.2309	3.7802E-01	2.2554E-02	6.3785E-01	1.3625E-01
LPA (14:0)	0.1212	0.0296	0.1372	0.1693	3.7903E-01	8.6180E-01	6.3785E-01	9.2762E-01
PGF1alpha/DGLA	0.1288	-0.3159	0.1466	0.2277	3.8138E-01	1.6960E-01	6.3785E-01	4.3187E-01
O-Acetyl-Ser	-0.1406	-0.1268	0.1601	0.2383	3.8142E-01	5.9610E-01	6.3785E-01	7.6631E-01
11-HETE	0.1618	0.1747	0.1855	0.2440	3.8464E-01	4.7594E-01	6.3930E-01	7.0652E-01
14-HDoHE/DHA	0.1640	0.3737	0.1888	0.2434	3.8661E-01	1.2877E-01	6.3930E-01	3.6301E-01
Citrulline/Ornithine	0.1462	-0.2313	0.1719	0.1554	3.9657E-01	1.4060E-01	6.5214E-01	3.8895E-01
18-HEPE	0.1499	0.5368	0.1780	0.2023	4.0158E-01	9.6236E-03	6.5672E-01	9.1002E-02
Sum HETEs	-0.1491	0.4345	0.1791	0.2771	4.0671E-01	1.2094E-01	6.6038E-01	3.5095E-01
8-iso-PGF3alpha/DGLA	-0.1112	-0.1762	0.1343	0.2088	4.0935E-01	4.0162E-01	6.6038E-01	6.6404E-01
9-HEPE/EPA	-0.1424	0.0761	0.1724	0.2402	4.1050E-01	7.5225E-01	6.6038E-01	8.6979E-01
Sum HEPEs	0.1393	0.5496	0.1703	0.2049	4.1492E-01	8.9328E-03	6.6387E-01	9.1002E-02
19,20-DiHDPa/19,20-EpDPE	0.1227	-0.1782	0.1512	0.2558	4.1887E-01	4.8806E-01	6.6659E-01	7.0816E-01
9-HOTe	-0.1365	0.1984	0.1700	0.2134	4.2336E-01	3.5540E-01	6.7013E-01	6.1162E-01
19,20-DiHDPa	-0.1361	0.4201	0.1716	0.2546	4.2926E-01	1.0282E-01	6.7388E-01	3.1703E-01
15-HETe/DGLA	0.1545	0.3535	0.1953	0.2573	4.3031E-01	1.7328E-01	6.7388E-01	4.3468E-01
Cys/Cystathionine	0.1413	-0.1810	0.1798	0.2630	4.3366E-01	4.9328E-01	6.7388E-01	7.1120E-01
12-KETE/12-HETE	0.1461	0.2049	0.1864	0.2586	4.3483E-01	4.3049E-01	6.7388E-01	6.7348E-01
Glucose	0.1379	0.1869	0.1777	0.2672	4.3909E-01	4.8685E-01	6.7694E-01	7.0816E-01
LA	0.1071	0.3623	0.1396	0.1664	4.4452E-01	3.2573E-02	6.8049E-01	1.7547E-01
7-HDoHE	-0.1083	0.2226	0.1422	0.2102	4.4771E-01	2.9293E-01	6.8049E-01	5.8201E-01
SIP (18:0)	0.1396	-0.2511	0.1837	0.2277	4.4878E-01	2.7342E-01	6.8049E-01	5.6994E-01
LPG (22:4)	-0.1233	0.1416	0.1629	0.2380	4.5060E-01	5.5376E-01	6.8049E-01	7.5189E-01
LPA (20:4)	-0.1247	-0.1172	0.1667	0.2148	4.5563E-01	5.8723E-01	6.8460E-01	7.6631E-01
Pro	0.1431	-0.2576	0.1935	0.2158	4.6099E-01	2.3697E-01	6.8916E-01	5.2738E-01
9-KODE	-0.1273	0.0174	0.1733	0.2156	4.6396E-01	9.3600E-01	6.9011E-01	9.6536E-01
O-PO3-EA	0.1587	0.0482	0.2228	0.2149	4.7782E-01	8.2296E-01	7.0538E-01	8.9888E-01
7-HDoHE/DHA	-0.1131	0.2036	0.1593	0.3001	4.7899E-01	4.9947E-01	7.0538E-01	7.1120E-01
Sum BA	0.1285	0.3844	0.1858	0.2859	4.9035E-01	1.8251E-01	7.1853E-01	4.5020E-01
15-HETE	0.1332	0.1935	0.1952	0.2475	4.9637E-01	4.3671E-01	7.2378E-01	6.7598E-01
cLPA (20:4)	-0.1159	-0.2155	0.1753	0.2212	5.0990E-01	3.3317E-01	7.3986E-01	5.9939E-01
Leu	-0.1254	-0.5076	0.1916	0.2354	5.1386E-01	3.5362E-02	7.4196E-01	1.8691E-01
Sarcosine	-0.1195	-0.3101	0.1838	0.2391	5.1700E-01	1.9837E-01	7.4288E-01	4.6601E-01
20-HETE	-0.1165	0.0297	0.1818	0.2486	5.2295E-01	9.0524E-01	7.4500E-01	9.6190E-01
EA	0.1052	0.2737	0.1654	0.1932	5.2580E-01	1.6046E-01	7.4500E-01	4.2790E-01
LPG (16:0)	0.1154	0.2339	0.1823	0.2319	5.2787E-01	3.1605E-01	7.4500E-01	5.9305E-01
5-aminolevulinic acid	-0.1174	-0.1270	0.1857	0.1983	5.2855E-01	5.2396E-01	7.4500E-01	7.2648E-01
18-HEPE/EPA	0.0893	0.2179	0.1471	0.2712	5.4478E-01	4.2408E-01	7.6424E-01	6.7152E-01
ETE	-0.1158	0.1283	0.1925	0.2570	5.4839E-01	6.1899E-01	7.6514E-01	7.8636E-01
2-aminoadipic acid	-0.0954	-0.1131	0.1593	0.2166	5.5059E-01	6.0292E-01	7.6514E-01	7.6924E-01
13-HDoHE/DHA	0.1018	0.3147	0.1742	0.2825	5.5988E-01	2.6866E-01	7.7440E-01	5.6679E-01
8-HETe/DGLA	0.1103	0.3079	0.1904	0.2498	5.6349E-01	2.2128E-01	7.7440E-01	5.0385E-01
Cys	0.0886	-0.3288	0.1536	0.2468	5.6510E-01	1.8657E-01	7.7440E-01	4.5391E-01
15-HETe	0.1130	0.4204	0.1990	0.2307	5.7105E-01	7.2175E-02	7.7894E-01	2.6573E-01
LPA (18:1)	-0.0962	0.1349	0.1723	0.2266	5.7744E-01	5.5370E-01	7.8405E-01	7.5189E-01
2,3-dinor-8-iso-PGF2alpha	0.1021	-0.2594	0.1871	0.2712	5.8633E-01	3.4201E-01	7.9248E-01	5.9939E-01
LPS (18:1)	0.1035	0.5203	0.1935	0.2674	5.9382E-01	5.5189E-02	7.9895E-01	2.3008E-01
LPA (20:5)	0.0903	0.4485	0.1709	0.2062	5.9816E-01	3.2604E-02	8.0007E-01	1.7547E-01

Chapter III

3-Met-His	0.1029	0.0648	0.1958	0.2600	6.0005E-01	8.0378E-01	8.0007E-01	8.9781E-01
LPG (22:6)	0.0614	0.2951	0.1187	0.1449	6.0616E-01	4.5258E-02	8.0458E-01	2.0610E-01
LPE (22:5)	-0.0980	-0.0123	0.1921	0.2025	6.1083E-01	9.5183E-01	8.0565E-01	9.6818E-01
cLPA (18:2)	-0.0850	-0.0075	0.1681	0.2075	6.1408E-01	9.7136E-01	8.0565E-01	9.8130E-01
14-HDoHE	0.1061	0.4756	0.2104	0.2488	6.1512E-01	5.9827E-02	8.0565E-01	2.3612E-01
LPG (18:0)	0.0850	0.1533	0.1788	0.1909	6.3532E-01	4.2424E-01	8.2024E-01	6.7152E-01
Coriolic acid	-0.0872	0.3013	0.1834	0.2264	6.3535E-01	1.8708E-01	8.2024E-01	4.5391E-01
TXB3	0.0800	0.1760	0.1684	0.2230	6.3573E-01	4.3230E-01	8.2024E-01	6.7348E-01
14,15-DiHETE	0.0677	0.5318	0.1438	0.2295	6.3864E-01	2.3211E-02	8.2024E-01	1.3741E-01
w3FA/w6FA	0.0533	0.1805	0.1137	0.1370	6.4012E-01	1.9152E-01	8.2024E-01	4.5724E-01
AA	-0.0867	0.1436	0.1938	0.2535	6.5533E-01	5.7273E-01	8.2820E-01	7.6307E-01
11beta-PGF2alpha	-0.0471	0.0280	0.1057	0.1710	6.5686E-01	8.7071E-01	8.2820E-01	9.3380E-01
12,13-DiHOME	-0.0601	0.0686	0.1350	0.1450	6.5690E-01	6.3757E-01	8.2820E-01	7.9967E-01
LPA (18:0)	0.0773	0.0736	0.1738	0.2179	6.5752E-01	7.3659E-01	8.2820E-01	8.6821E-01
LPI (18:2)	0.0645	0.5167	0.1494	0.1657	6.6685E-01	2.5302E-03	8.3028E-01	4.1607E-02
15-HEPE/EPA	-0.0685	0.1204	0.1627	0.2271	6.7419E-01	5.9738E-01	8.3028E-01	7.6631E-01
Sum iPs	0.0674	-0.0243	0.1604	0.2363	6.7492E-01	9.1826E-01	8.3028E-01	9.6536E-01
5-iPF2alpha-VI/AA	0.0806	0.2199	0.1936	0.2265	6.7797E-01	3.3471E-01	8.3028E-01	5.9939E-01
8-HDoHE	-0.0587	0.2054	0.1411	0.2067	6.7837E-01	3.2330E-01	8.3028E-01	5.9628E-01
16-HDoHE	-0.0603	0.3799	0.1452	0.1891	6.7877E-01	4.7991E-02	8.3028E-01	2.1202E-01
EPA	0.0465	0.3446	0.1121	0.1360	6.7881E-01	1.3195E-02	8.3028E-01	1.1074E-01
10-HDoHE	-0.0783	0.3662	0.1942	0.2164	6.8739E-01	9.4604E-02	8.3466E-01	3.0438E-01
11-HDoHE/DHA	0.0789	0.4272	0.1968	0.2473	6.8929E-01	8.8022E-02	8.3466E-01	2.8838E-01
cLPA (14:0)	-0.0522	-0.3557	0.1309	0.1669	6.9085E-01	3.6335E-02	8.3466E-01	1.8868E-01
17-HDoHE	-0.0653	0.4224	0.1781	0.2000	7.1468E-01	3.7807E-02	8.5682E-01	1.8968E-01
PGA2	0.0659	0.0434	0.1799	0.1879	7.1498E-01	8.1823E-01	8.5682E-01	8.9888E-01
8-HETE	0.0719	0.3935	0.2031	0.2351	7.2403E-01	9.8166E-02	8.6417E-01	3.0912E-01
Carnosine	-0.0528	-0.3420	0.1559	0.1881	7.3546E-01	7.2717E-02	8.7428E-01	2.6573E-01
HomoCys	-0.0482	-0.2008	0.1513	0.2829	7.5062E-01	4.7983E-01	8.8874E-01	7.0652E-01
LPG (18:3)	-0.0418	0.1305	0.1365	0.1752	7.5981E-01	4.5837E-01	8.9631E-01	6.9554E-01
13,14-dihydro-15-keto-PGF2alpha	-0.0565	-0.0442	0.1894	0.2259	7.6594E-01	8.4535E-01	8.9922E-01	9.1322E-01
17-HDoHE/DHA	-0.0540	0.5192	0.1858	0.2716	7.7171E-01	5.9500E-02	8.9922E-01	2.3612E-01
PGA2/AA	0.0538	0.0204	0.1884	0.1869	7.7573E-01	9.1339E-01	8.9922E-01	9.6536E-01
LPS (20:4)	-0.0422	-0.1402	0.1497	0.1847	7.7845E-01	4.5023E-01	8.9922E-01	6.8694E-01
cLPA (18:1)	-0.0483	-0.0946	0.1725	0.2065	7.8016E-01	6.4805E-01	8.9922E-01	8.0938E-01
TXB3/EPA	0.0411	-0.0202	0.1473	0.2428	7.8074E-01	9.3390E-01	8.9922E-01	9.6536E-01
10-HDoHE/DHA	-0.0514	0.3312	0.1907	0.2514	7.8780E-01	1.9155E-01	9.0383E-01	4.5724E-01
LPI (22:6)	0.0543	0.2038	0.2055	0.1835	7.9203E-01	2.6999E-01	9.0518E-01	5.6679E-01
LPE (16:1)	-0.0441	-0.5147	0.1701	0.2135	7.9605E-01	1.8733E-02	9.0627E-01	1.3205E-01
16-HDoHE/DHA	-0.0426	0.5152	0.1672	0.2853	7.9941E-01	7.4759E-02	9.0661E-01	2.6780E-01
Anserine	0.0509	-0.3701	0.2058	0.2052	8.0490E-01	7.5093E-02	9.0935E-01	2.6780E-01
Cystathionine/HomoCys	-0.0408	0.0637	0.1703	0.2458	8.1113E-01	7.9623E-01	9.1291E-01	8.9614E-01
5-iPF2alpha-VI	-0.0346	0.4349	0.1603	0.2451	8.2937E-01	8.0189E-02	9.2990E-01	2.7925E-01
DHA	-0.0328	0.1111	0.1559	0.1814	8.3397E-01	5.4195E-01	9.3153E-01	7.4268E-01
Sum HODEs	-0.0352	0.2964	0.1754	0.2297	8.4143E-01	2.0064E-01	9.3290E-01	4.6709E-01
THDCA	0.0278	0.1284	0.1389	0.1614	8.4164E-01	4.2864E-01	9.3290E-01	6.7348E-01
11beta-PGF2alpha/AA	-0.0261	-0.0187	0.1330	0.2016	8.4465E-01	9.2626E-01	9.3290E-01	9.6536E-01
LPG (16:1)	-0.0332	-0.1690	0.1893	0.2212	8.6117E-01	4.4743E-01	9.4436E-01	6.8622E-01
LPA (16:1)	0.0290	-0.0164	0.1657	0.2263	8.6141E-01	9.4228E-01	9.4436E-01	9.6715E-01
GCDCa	0.0221	0.0255	0.1473	0.2004	8.8116E-01	8.9921E-01	9.5777E-01	9.6089E-01
5-KETE	0.0262	0.3428	0.1773	0.2614	8.8296E-01	1.9358E-01	9.5777E-01	4.5841E-01
15-HEPE	0.0228	0.5168	0.1557	0.1929	8.8409E-01	8.9713E-03	9.5777E-01	9.1002E-02
13,14-dihydro-15-keto-PGF2alpha/AA	0.0290	-0.1567	0.2031	0.2204	8.8659E-01	4.7917E-01	9.5777E-01	7.0652E-01
9-HODE	0.0228	0.2839	0.1671	0.2361	8.9150E-01	2.3264E-01	9.5905E-01	5.2168E-01
20-HDoHE	-0.0233	0.4728	0.1747	0.2128	8.9425E-01	2.9104E-02	9.5905E-01	1.6254E-01
LPA (22:5)	-0.0232	0.2170	0.1889	0.2008	9.0235E-01	2.8359E-01	9.6081E-01	5.8201E-01
FA (18:0)	-0.0239	-0.1510	0.1945	0.2233	9.0239E-01	5.0098E-01	9.6081E-01	7.1120E-01
17,18-DiHETE	0.0176	0.2988	0.1549	0.2615	9.0973E-01	2.5654E-01	9.6517E-01	5.5428E-01
Sum HDoHEs	-0.0189	0.4726	0.2023	0.2292	9.2564E-01	4.2624E-02	9.7736E-01	2.0091E-01
5-OH-Trp	0.0156	-0.4505	0.1724	0.2745	9.2783E-01	1.0496E-01	9.7736E-01	3.1703E-01
20-HETE/AA	-0.0157	-0.2149	0.1917	0.2227	9.3469E-01	3.3831E-01	9.8103E-01	5.9939E-01
Clupanodonic acid	-0.0118	0.1869	0.1616	0.1851	9.4211E-01	3.1574E-01	9.8103E-01	5.9305E-01
Sum DiHETEs	0.0098	0.4121	0.1407	0.2620	9.4459E-01	1.2048E-01	9.8103E-01	3.5095E-01
LPI (20:4)	-0.0123	0.1082	0.1834	0.1919	9.4671E-01	5.7426E-01	9.8103E-01	7.6307E-01
LPA (16:0)	0.0097	0.0754	0.1586	0.2105	9.5119E-01	7.2110E-01	9.8103E-01	8.5721E-01
20-HDoHE/DHA	0.0108	0.4501	0.1766	0.2461	9.5121E-01	7.1192E-02	9.8103E-01	2.6573E-01
8-HDoHE/DHA	-0.0081	0.1962	0.1589	0.2926	9.5920E-01	5.0457E-01	9.8471E-01	7.1120E-01
13-HDoHE	0.0071	0.2983	0.1513	0.2037	9.6246E-01	1.4714E-01	9.8471E-01	4.0327E-01

9-HEPE	-0.0067	0.4238	0.1514	0.1784	9.6475E-01	1.9991E-02	9.8471E-01	1.3296E-01
DGLA	-0.0079	0.1247	0.2055	0.2348	9.6942E-01	5.9697E-01	9.8483E-01	7.6631E-01
Sum HETrEs	-0.0061	0.3196	0.1971	0.2295	9.7547E-01	1.6774E-01	9.8483E-01	4.3175E-01
PAF 18(2)	0.0044	0.3386	0.1592	0.1963	9.7809E-01	8.8380E-02	9.8483E-01	2.8838E-01
11-HDoHE	0.0052	0.4085	0.1900	0.2132	9.7818E-01	5.8987E-02	9.8483E-01	2.3612E-01
AEA	-0.0021	0.4139	0.1442	0.1713	9.8824E-01	1.8737E-02	9.9159E-01	1.3205E-01
ALA	0.0008	0.1481	0.1306	0.1693	9.9517E-01	3.8425E-01	9.9517E-01	6.4259E-01

Table S10: Linear mixed-effect model results of the pathogen-stratified "Sepsis" models

Metabolite	Estimate Gram-Negative	Estimate Gram-Positive	Standard Error Gram-Negative	Standard Error Gram-Positive	p-value Gram-Negative	p-value Gram-Positive	Adjusted p-value Gram-Negative	Adjusted p-value Gram-Positive
Thr	-0.8784	-0.7352	0.2267	0.1829	1.6179E-04	8.9544E-05	2.3871E-02	3.0999E-03
4-OH-Pro	-0.9198	-0.5925	0.2420	0.1936	2.1229E-04	2.6036E-03	2.3871E-02	2.6575E-02
Citrulline	-0.8020	-0.3369	0.2168	0.1878	3.1446E-04	7.4757E-02	2.3871E-02	2.1353E-01
3-Methoxytyrosine	-0.9001	-0.4100	0.2457	0.1984	3.5043E-04	4.0379E-02	2.3871E-02	1.5459E-01
PGE1	1.0303	0.0000	0.2843	0.2410	4.0323E-04	9.9999E-01	2.3871E-02	9.9999E-01
Arg	-0.9861	-0.5093	0.2804	0.2208	5.8583E-04	2.2389E-02	2.6866E-02	1.1627E-01
Sum OG	-0.9254	-0.4606	0.2668	0.2197	6.9224E-04	3.7640E-02	2.6866E-02	1.4855E-01
PGE1/DGLA	1.0184	-0.0848	0.2947	0.2384	7.2610E-04	7.2244E-01	2.6866E-02	8.6704E-01
LPS (18:0)	0.8336	0.9423	0.2489	0.2037	1.0393E-03	1.8710E-06	3.2864E-02	5.9617E-04
SDMA	-0.8040	-0.2686	0.2434	0.1893	1.2050E-03	5.7199E-01	3.2864E-02	3.7114E-01
OH-Lys	-0.8509	-0.6635	0.2595	0.2083	1.3070E-03	1.7459E-03	3.2864E-02	2.1202E-02
PGE2/AA	0.9243	0.2441	0.2824	0.2160	1.3323E-03	2.6020E-01	3.2864E-02	5.2393E-01
PGE2	0.9354	0.0077	0.2927	0.2255	1.7130E-03	9.7290E-01	3.9005E-02	9.9993E-01
ADMA	-0.8333	-0.7811	0.2649	0.2069	2.0317E-03	2.2662E-04	4.2955E-02	4.7914E-03
Gln	-0.8708	-0.5965	0.2916	0.2193	3.3368E-03	7.2583E-03	6.4163E-02	4.8829E-02
GABA	0.8181	0.0781	0.2753	0.2269	3.4683E-03	7.3123E-01	6.4163E-02	8.6704E-01
Trimethyl-Lys	-0.7959	-0.5714	0.2727	0.1992	4.1226E-03	4.1713E-03	6.7449E-02	3.6713E-02
Tyr	-0.6171	-0.6790	0.2142	0.1736	4.5661E-03	1.3611E-04	6.7449E-02	3.3574E-03
AAA	-0.6864	-0.7477	0.2398	0.1881	4.8332E-03	1.0615E-04	6.7449E-02	3.0999E-03
5-HT/Trp	0.7940	0.6047	0.2777	0.2185	4.9004E-03	6.3436E-03	6.7449E-02	4.6461E-02
PGF2alpha	0.8678	0.0020	0.3041	0.2241	4.9747E-03	9.9284E-01	6.7449E-02	9.9999E-01
Phe/Tyr	0.5162	0.5873	0.1811	0.1535	5.0131E-03	1.8650E-04	6.7449E-02	4.2463E-03
Sum PGs	0.8443	0.0927	0.2989	0.2272	5.4037E-03	6.8393E-01	6.9544E-02	8.6175E-01
g-Glu-Gln	-0.8148	-0.7859	0.2908	0.2243	5.8069E-03	5.9628E-04	7.1619E-02	1.0382E-02
PGF2alpha/AA	0.8106	0.2726	0.2918	0.2092	6.1973E-03	1.9439E-01	7.3376E-02	4.2157E-01
Lys	-0.7307	-0.5022	0.2728	0.2238	8.2557E-03	2.6199E-02	9.3988E-02	1.2713E-01
LPI (18:0)	0.6552	0.5448	0.2456	0.1818	8.5803E-03	3.2053E-03	9.4066E-02	2.9649E-02
Sum LG	-0.6361	-0.0996	0.2421	0.1944	9.5360E-03	6.0900E-01	1.0081E-01	8.2658E-01
Glu/GABA	-0.6684	-0.1898	0.2562	0.2043	1.0089E-02	3.5427E-01	1.0298E-01	6.3554E-01
12,13-EpOME/LA	-0.6841	-0.4041	0.2645	0.2109	1.0737E-02	5.7229E-02	1.0594E-01	1.9471E-01
LPI (18:1)	0.6472	-0.0318	0.2541	0.1916	1.2015E-02	8.6850E-01	1.1472E-01	9.4167E-01
4-OH-Pro/Pro	-0.6379	-0.3725	0.2557	0.2080	1.3771E-02	7.5147E-02	1.2738E-01	2.1353E-01
Asn	-0.4901	-0.4414	0.1984	0.1303	1.4848E-02	8.9018E-04	1.3318E-01	1.3868E-02
Ornithine	-0.6143	-0.4689	0.2505	0.2017	1.5417E-02	2.1312E-02	1.3422E-01	1.1509E-01
Met	-0.6331	-0.5387	0.2728	0.2246	2.1692E-02	1.7626E-02	1.8080E-01	1.0230E-01
Homoserine	-0.6176	-0.6143	0.2667	0.2131	2.1989E-02	4.4919E-03	1.8080E-01	3.5935E-02
9-KODE/9-HODE	-0.6027	-0.4231	0.2615	0.2005	2.2669E-02	3.6489E-02	1.8135E-01	1.4855E-01
Gln/Glu	-0.6847	-0.4216	0.3007	0.2363	2.4486E-02	7.6497E-02	1.9073E-01	2.1353E-01
Trp	-0.4860	-1.0291	0.2152	0.1645	2.5502E-02	3.5967E-09	1.9356E-01	1.0646E-06
5-HT	0.6209	0.2675	0.2764	0.2211	2.6252E-02	2.2816E-01	1.9427E-01	4.7197E-01
Sum AG	-0.5706	-0.2135	0.2577	0.2037	2.8394E-02	2.9618E-01	2.0499E-01	5.7460E-01
12-HEPE/EPA	0.6465	-0.0220	0.2939	0.2400	2.9484E-02	9.2694E-01	2.0779E-01	9.6611E-01
Kyn	-0.5676	-0.4027	0.2593	0.2115	3.0192E-02	5.8733E-02	2.0783E-01	1.9624E-01
Saccharopine	-0.6251	-0.6821	0.2906	0.2275	3.3173E-02	3.1576E-03	2.2316E-01	2.9649E-02
Sum KETEs	0.6325	0.3143	0.2967	0.2358	3.4766E-02	1.8453E-01	2.2371E-01	4.0761E-01
BCAA/Tyr	0.3775	0.4481	0.1785	0.1515	3.6239E-02	3.5692E-03	2.2371E-01	3.1987E-02
Arg/Lys	-0.6156	-0.2691	0.2917	0.2256	3.6604E-02	2.3474E-01	2.2371E-01	4.7920E-01
12-HEPE	0.5622	0.0685	0.2671	0.2129	3.7033E-02	7.4817E-01	2.2371E-01	8.6846E-01
delta-17,6-keto-PGF1alpha/EPA	0.5382	0.2597	0.2555	0.1978	3.7033E-02	1.9117E-01	2.2371E-01	4.1916E-01
Ser	-0.5947	-0.4004	0.2843	0.2288	3.8232E-02	8.2076E-02	2.2634E-01	2.2705E-01
Putrescine	0.6068	0.3219	0.2925	0.2222	3.9834E-02	1.4949E-01	2.3119E-01	3.5684E-01
LPG (20:3)	-0.5776	-0.4450	0.2796	0.2340	4.0712E-02	5.9004E-02	2.3175E-01	1.9624E-01
Gly-Pro	-0.5000	-0.5419	0.2453	0.1930	4.3341E-02	5.6003E-03	2.4074E-01	4.2505E-02
LPE (22:4)	-0.5032	-0.3712	0.2475	0.2008	4.3920E-02	6.6375E-02	2.4074E-01	2.1028E-01
Sphinganine 18.0	0.5920	0.4452	0.2948	0.2417	4.6579E-02	6.7389E-02	2.5068E-01	2.1028E-01
Carnosine	-0.4525	0.2035	0.2269	0.1675	4.8136E-02	2.2613E-01	2.5443E-01	4.7137E-01
14-HDoHE/DHA	0.5797	0.0345	0.2974	0.2378	5.3288E-02	8.8472E-01	2.7673E-01	9.4347E-01

Chapter III

2-aminoadipic acid	-0.4642	-0.1778	0.2395	0.1928	5.4552E-02	3.5765E-01	2.7795E-01	6.3773E-01
5-KETE/5-HETE	0.5258	0.8328	0.2727	0.2282	5.6018E-02	3.5915E-04	2.7795E-01	7.0872E-03
12,13-EpOME	-0.5368	-0.2026	0.2790	0.2242	5.6342E-02	3.6755E-01	2.7795E-01	6.4759E-01
LPE (18:0)	0.4530	0.4412	0.2379	0.1861	5.8918E-02	1.8983E-02	2.7976E-01	1.0806E-01
LPG (20:4)	-0.4702	-0.2094	0.2474	0.1957	5.9342E-02	2.8624E-01	2.7976E-01	5.6175E-01
14-HDoHE	0.5956	0.0108	0.3137	0.2550	5.9722E-02	9.6639E-01	2.7976E-01	9.9669E-01
12-HETE/AA	0.5822	0.0001	0.3089	0.2513	6.1584E-02	9.9980E-01	2.7976E-01	9.9999E-01
LPE (16:0)	0.4636	0.6495	0.2467	0.1958	6.2221E-02	1.1299E-03	2.7976E-01	1.6723E-02
12-KETE	0.5200	0.0963	0.2768	0.2258	6.2380E-02	6.7024E-01	2.7976E-01	8.5673E-01
12-HETE	0.5882	-0.1971	0.3150	0.2579	6.3950E-02	4.4570E-01	2.8252E-01	7.2092E-01
Anserine	-0.4452	0.3505	0.2408	0.2334	6.6593E-02	1.3512E-01	2.8962E-01	3.2941E-01
LPG (18:1)	-0.5072	-0.4781	0.2756	0.2271	6.7786E-02	3.6870E-02	2.8962E-01	1.4855E-01
LPI (16:0)	0.4899	0.5951	0.2673	0.2024	6.8883E-02	3.7270E-03	2.8962E-01	3.1987E-02
Val	-0.4923	-0.3959	0.2691	0.2190	6.9471E-02	7.2576E-02	2.8962E-01	2.1353E-01
PGF1alpha	0.3328	0.1457	0.1850	0.1406	7.4091E-02	3.0148E-01	3.0460E-01	5.7572E-01
Sum SBA	-0.5311	-0.3304	0.2991	0.2368	7.7964E-02	1.6489E-01	3.1125E-01	3.8410E-01
BCAA/AAA	0.3360	0.3393	0.1895	0.1614	7.8333E-02	3.7148E-02	3.1125E-01	1.4855E-01
BCAA	-0.5094	-0.5000	0.2878	0.2352	7.8863E-02	3.5068E-02	3.1125E-01	1.4855E-01
11,12-DiHETrE	-0.4275	-0.7575	0.2452	0.1898	8.3320E-02	1.0048E-04	3.2146E-01	3.0999E-03
TLCA-3S	-0.5148	-0.4929	0.2955	0.2332	8.3622E-02	3.6111E-02	3.2146E-01	1.4855E-01
delta-17,6-keto-PGF1alpha	0.4840	0.3169	0.2805	0.2215	8.6649E-02	1.5458E-01	3.2551E-01	3.6605E-01
GLA	-0.4458	-0.5781	0.2586	0.2097	8.6875E-02	6.5247E-03	3.2551E-01	4.6461E-02
Sum PBA	0.5112	-0.0310	0.2977	0.2444	8.8069E-02	8.9919E-01	3.2585E-01	9.5057E-01
LCA	-0.4363	-0.6617	0.2583	0.2146	9.3379E-02	2.4202E-03	3.3921E-01	2.6245E-02
Ile	-0.5034	-0.5722	0.2985	0.2458	9.3970E-02	2.1200E-02	3.3921E-01	1.1509E-01
Sum HEPeS	0.4355	0.1582	0.2609	0.2099	9.7288E-02	4.5217E-01	3.4696E-01	7.2346E-01
LPA (20:5)	0.4143	-0.2730	0.2540	0.2041	1.0503E-01	1.8290E-01	3.7010E-01	4.0761E-01
Cystathionine	-0.3801	-0.1324	0.2355	0.1843	1.0889E-01	4.7365E-01	3.7920E-01	7.4574E-01
HomoCys	-0.4865	-0.1659	0.3044	0.2402	1.1215E-01	4.9091E-01	3.8253E-01	7.6250E-01
Ala	-0.4369	-0.6368	0.2743	0.2313	1.1346E-01	6.5924E-03	3.8253E-01	4.6461E-02
LPA (14:0)	0.3115	-0.3132	0.1960	0.1567	1.1418E-01	4.7344E-02	3.8253E-01	1.6784E-01
LPE (20:5)	-0.4337	-0.3700	0.2735	0.2224	1.1502E-01	9.8221E-02	3.8253E-01	2.6430E-01
Sum TxS	0.4508	-0.0372	0.2856	0.2317	1.1659E-01	8.7282E-01	3.8346E-01	9.4290E-01
Ornithine/Arg	0.4685	0.0905	0.3034	0.2306	1.2483E-01	6.9509E-01	4.0605E-01	8.6175E-01
TXB2	0.4122	-0.1246	0.2702	0.2124	1.2932E-01	5.5841E-01	4.0836E-01	8.0080E-01
S-Methyl-Cys	-0.3913	-0.3883	0.2569	0.2175	1.2997E-01	7.6125E-02	4.0836E-01	2.1353E-01
Sum BA	0.4852	0.0736	0.3195	0.2509	1.3106E-01	7.6964E-01	4.0836E-01	8.8990E-01
g-Glu-Ala	-0.4100	-0.5786	0.2703	0.2184	1.3154E-01	8.8919E-03	4.0836E-01	5.8489E-02
CA	0.3907	-0.0526	0.2582	0.2123	1.3244E-01	8.0472E-01	4.0836E-01	9.1605E-01
PGF1alpha/DGLA	0.3477	0.1080	0.2331	0.1841	1.3810E-01	5.5835E-01	4.2141E-01	8.0080E-01
HCA	0.3857	0.0997	0.2612	0.2141	1.4195E-01	6.4207E-01	4.2795E-01	8.3723E-01
15-HETE/AA	0.4288	0.0160	0.2927	0.2318	1.4516E-01	9.4498E-01	4.2795E-01	9.8146E-01
8-HETrE/DGLA	0.4324	0.0397	0.2961	0.2356	1.4637E-01	8.6626E-01	4.2795E-01	9.4167E-01
LPA (16:0)	0.3374	-0.3592	0.2316	0.1807	1.4747E-01	4.8558E-02	4.2795E-01	1.6910E-01
Cortisol	0.3815	0.5604	0.2622	0.2137	1.4783E-01	9.5896E-03	4.2795E-01	6.1707E-02
THDCA	-0.2822	0.3664	0.1946	0.1522	1.4910E-01	1.7276E-02	4.2795E-01	1.0227E-01
Arg/ADMA	-0.4316	0.0332	0.2985	0.2313	1.5036E-01	8.8610E-01	4.2795E-01	9.4347E-01
TCA	-0.3007	-0.1594	0.2115	0.1842	1.5742E-01	3.8832E-01	4.3440E-01	6.6827E-01
Gly	-0.3671	-0.3478	0.2596	0.2110	1.5949E-01	1.0121E-01	4.3440E-01	2.6989E-01
LPE (18:2)	-0.3638	-0.4506	0.2575	0.2041	1.5990E-01	2.8705E-02	4.3440E-01	1.3276E-01
LPE (20:4)	-0.3437	-0.6093	0.2453	0.2000	1.6326E-01	2.7174E-03	4.3440E-01	2.6811E-02
TXB3	0.3708	-0.1121	0.2658	0.2120	1.6519E-01	5.9787E-01	4.3440E-01	8.1931E-01
Cys	-0.3766	-0.0924	0.2707	0.2174	1.6641E-01	6.7149E-01	4.3440E-01	8.5673E-01
12-HHTrE	0.3568	-0.0880	0.2589	0.2013	1.7036E-01	6.6262E-01	4.3440E-01	8.5276E-01
GCA	-0.4021	-0.3961	0.2926	0.2339	1.7157E-01	9.2348E-02	4.3440E-01	2.5310E-01
His	-0.3599	-0.3795	0.2624	0.2084	1.7253E-01	7.0606E-02	4.3440E-01	2.1353E-01
LPI (16:1)	0.3646	-0.2269	0.2675	0.2121	1.7525E-01	2.8657E-01	4.3440E-01	5.6175E-01
15-HETrE/DGLA	0.4176	0.0685	0.3073	0.2451	1.7622E-01	7.8008E-01	4.3440E-01	8.9541E-01
3-AIBA	-0.2490	0.1893	0.1832	0.1536	1.7664E-01	2.1990E-01	4.3440E-01	4.6493E-01
Sum DIHETrEs	-0.3382	-0.9248	0.2494	0.2004	1.7726E-01	8.0564E-06	4.3440E-01	5.9617E-04
TXB2/AA	0.3581	0.0693	0.2653	0.2086	1.7927E-01	7.4022E-01	4.3440E-01	8.6704E-01
5-KETE	0.4351	0.0614	0.3224	0.2560	1.7929E-01	8.1065E-01	4.3440E-01	9.1605E-01
15-HETE	0.4105	-0.3022	0.3050	0.2446	1.8048E-01	2.1840E-01	4.3440E-01	4.6493E-01
Sarcosine	-0.3701	-0.2781	0.2753	0.2276	1.8102E-01	2.2369E-01	4.3440E-01	4.6958E-01
5-HETE/AA	-0.3176	-0.4913	0.2366	0.1983	1.8175E-01	1.4252E-02	4.3440E-01	8.6092E-02
TXB3/EPA	0.3271	-0.3124	0.2442	0.1995	1.8250E-01	1.1935E-01	4.3440E-01	3.0989E-01
Sum HDoHEs	0.3988	0.0275	0.2979	0.2385	1.8290E-01	9.0840E-01	4.3440E-01	9.5584E-01
12-KETE/12-HETE	0.3942	0.4106	0.2949	0.2230	1.8345E-01	6.7489E-02	4.3440E-01	2.1028E-01
AEA	0.2880	0.0673	0.2178	0.1759	1.8851E-01	7.0254E-01	4.4286E-01	8.6175E-01
LPI (18:2)	0.2798	0.0369	0.2153	0.1673	1.9589E-01	8.2576E-01	4.5655E-01	9.1838E-01

Diagnosis of Late-Onset Sepsis

12,13-DiHOME/12,13-EpOME	0.2470	0.0926	0.1932	0.1582	2.0308E-01	5.5947E-01	4.6756E-01	8.0080E-01
LPS (18:2)	0.2895	0.1679	0.2269	0.2033	2.0417E-01	4.1015E-01	4.6756E-01	6.9373E-01
LPI (22:4)	-0.3341	-0.3899	0.2626	0.2151	2.0535E-01	7.1725E-02	4.6756E-01	2.1353E-01
TXB1	0.3570	0.0455	0.2827	0.2191	2.0875E-01	8.3568E-01	4.7167E-01	9.2299E-01
11-HDoHE/DHA	0.3820	0.2325	0.3068	0.2421	2.1514E-01	3.3823E-01	4.7909E-01	6.1968E-01
11-HDoHE	0.3467	0.1186	0.2793	0.2228	2.1658E-01	5.9547E-01	4.7909E-01	8.1931E-01
LPG (18:2)	-0.3020	-0.1242	0.2448	0.1956	2.1935E-01	5.2626E-01	4.7909E-01	7.8150E-01
LPA (20:3)	0.2870	-0.5999	0.2339	0.1910	2.2181E-01	2.0125E-03	4.7909E-01	2.2911E-02
TXB1/DGLA	0.3492	0.0874	0.2849	0.2257	2.2225E-01	6.9905E-01	4.7909E-01	8.6175E-01
LPE (20:3)	-0.2926	-0.8124	0.2389	0.2042	2.2258E-01	1.0499E-04	4.7909E-01	3.0999E-03
12-HHTrE/AA	0.3061	0.0753	0.2514	0.1944	2.2548E-01	6.9912E-01	4.7909E-01	8.6175E-01
LPA (22:5)	0.3437	-0.3996	0.2825	0.2232	2.2570E-01	7.5263E-02	4.7909E-01	2.1353E-01
Sphingosine18.1	0.3701	0.1371	0.3053	0.2435	2.2745E-01	5.7413E-01	4.7909E-01	8.0541E-01
LPE (22:6)	-0.3274	-0.7403	0.2711	0.2283	2.2912E-01	1.4408E-03	4.7909E-01	2.0309E-02
Leu	-0.3655	-0.5328	0.3030	0.2462	2.2983E-01	3.1975E-02	4.7909E-01	1.4173E-01
8,9-DiHETrE	-0.3057	-0.8924	0.2553	0.2094	2.3315E-01	3.4627E-05	4.8260E-01	1.7083E-03
LPA (18:2)	0.2715	-0.4148	0.2297	0.1876	2.3932E-01	2.8489E-02	4.8693E-01	1.3276E-01
LPA (18:0)	0.3003	-0.1155	0.2549	0.1986	2.4077E-01	5.6175E-01	4.8693E-01	8.0080E-01
LPA (22:6)	0.3193	-0.6454	0.2711	0.2197	2.4078E-01	3.7943E-03	4.8693E-01	3.1987E-02
8-HETrE	0.3540	-0.0865	0.3020	0.2421	2.4317E-01	7.2147E-01	4.8693E-01	8.6704E-01
GCDA	-0.2704	-0.1627	0.2309	0.1809	2.4346E-01	3.6991E-01	4.8693E-01	6.4789E-01
14,15-DiHETrE	-0.3003	-0.6512	0.2590	0.2050	2.4818E-01	1.7907E-03	4.9303E-01	2.1202E-02
cLPA (16:1)	-0.3137	-0.6950	0.2718	0.2162	2.5039E-01	1.5848E-03	4.9409E-01	2.0396E-02
11,12-EpETrE/AA	-0.2891	-0.0958	0.2577	0.2180	2.6376E-01	6.6106E-01	5.1705E-01	8.5276E-01
11-HETE	0.3241	-0.1920	0.3006	0.2352	2.8277E-01	4.1556E-01	5.4708E-01	6.9494E-01
LPE (14:0)	0.2895	-0.0485	0.2708	0.2233	2.8677E-01	8.2841E-01	5.4708E-01	9.1838E-01
LPA (18:1)	0.2789	-0.4109	0.2613	0.2058	2.8774E-01	4.7630E-02	5.4708E-01	1.6784E-01
11-HETE/AA	0.3284	0.1550	0.3079	0.2346	2.8811E-01	5.0982E-01	5.4708E-01	7.6993E-01
15-HETrE	0.3221	-0.0794	0.3022	0.2403	2.8832E-01	7.4168E-01	5.4708E-01	8.6704E-01
LPI (14:0)	0.2392	-0.2952	0.2278	0.1831	2.9540E-01	1.0898E-01	5.5498E-01	2.8803E-01
DHEA	0.1746	0.2594	0.1675	0.1283	2.9922E-01	4.4877E-02	5.5498E-01	1.6400E-01
DPA	-0.2933	-0.3524	0.2815	0.2326	2.9925E-01	1.3182E-01	5.5498E-01	3.2645E-01
19,20-EpDPE/DHA	-0.2285	0.1110	0.2197	0.2126	2.9999E-01	6.0232E-01	5.5498E-01	8.2160E-01
5-HEPE/EPA	-0.1846	-0.3299	0.1821	0.1464	3.1243E-01	2.5613E-02	5.7441E-01	1.2636E-01
Tau	0.2662	0.2319	0.2734	0.2218	3.3201E-01	2.9751E-01	6.0664E-01	5.7460E-01
LPS (18:1)	0.2943	-0.1194	0.3039	0.2395	3.3450E-01	6.1885E-01	6.0744E-01	8.2658E-01
Sum HETrEs	0.2683	-0.1716	0.2870	0.2342	3.3137E-01	4.6480E-01	6.3418E-01	7.3968E-01
LPG (22:4)	-0.2535	-0.1727	0.2769	0.2236	3.6154E-01	4.4104E-01	6.4054E-01	7.2092E-01
3-Met-His	0.2633	-0.1372	0.2882	0.2031	3.6237E-01	5.0045E-01	6.4054E-01	7.6501E-01
Homocitrulline	-0.2210	-0.4908	0.2423	0.1902	3.6338E-01	1.0792E-02	6.4054E-01	6.6554E-02
8,12-iso-iPF2alpha-VI/AA	-0.2537	-0.1710	0.2792	0.2232	3.6506E-01	4.4493E-01	6.4054E-01	7.2092E-01
Kyn/Trp	-0.2293	0.3904	0.2527	0.2171	3.6571E-01	7.4002E-02	6.4054E-01	2.1353E-01
Met-SO	-0.2497	-0.4677	0.2800	0.2153	3.7409E-01	3.1332E-02	6.5136E-01	1.4173E-01
15-HEPE	0.1973	0.1093	0.2260	0.1906	3.8413E-01	5.6731E-01	6.6493E-01	8.0080E-01
18-HEPE/EPA	0.2404	0.1056	0.2785	0.2234	3.8963E-01	6.3722E-01	6.6757E-01	8.3458E-01
10-HDoHE	0.2456	-0.0456	0.2879	0.2304	3.9500E-01	8.4330E-01	6.6757E-01	9.2795E-01
3-Methoxytyramine	0.2363	0.2645	0.2780	0.2537	3.9692E-01	2.9895E-01	6.6757E-01	5.7460E-01
5-HETrE	-0.2206	-0.3555	0.2602	0.2113	3.9807E-01	9.4478E-02	6.6757E-01	2.5656E-01
cLPA (18:0)	0.2230	0.0025	0.2641	0.2086	3.9977E-01	9.9053E-01	6.6757E-01	9.9999E-01
Pro	-0.2335	-0.2184	0.2778	0.2328	4.0198E-01	3.4969E-01	6.6757E-01	6.3456E-01
8-iso-PGF3alpha	-0.1547	0.0789	0.1842	0.1612	4.0309E-01	6.2552E-01	6.6757E-01	8.2658E-01
11beta-PGF2alpha	-0.1620	0.0336	0.1932	0.1453	4.0370E-01	8.1764E-01	6.6757E-01	9.1675E-01
20-HDoHE/DHA	0.2366	0.1624	0.2846	0.2282	4.0708E-01	4.7773E-01	6.6942E-01	7.4819E-01
LPS (22:4)	0.2248	0.4063	0.2720	0.2254	4.0997E-01	7.3404E-02	6.7045E-01	2.1353E-01
LPG (18:3)	-0.1717	-0.1567	0.2095	0.1630	4.1372E-01	3.3800E-01	6.7287E-01	6.1968E-01
Glutathione	0.2087	0.1778	0.2559	0.2151	4.1613E-01	4.0969E-01	6.7308E-01	6.9373E-01
PAF 16(0)	-0.2438	-0.3554	0.3032	0.2377	4.2269E-01	1.3689E-01	6.7642E-01	3.2941E-01
Asp	0.2354	-0.1495	0.2937	0.2325	4.2412E-01	5.2130E-01	6.7642E-01	7.8150E-01
20-HDoHE	0.2232	0.0915	0.2790	0.2187	4.2505E-01	6.7644E-01	6.7642E-01	8.5933E-01
18-HEPE	0.2135	0.2010	0.2721	0.2096	4.3410E-01	3.3915E-01	6.8714E-01	6.1968E-01
9-HODE	0.2086	0.1297	0.2675	0.2260	4.3682E-01	5.6687E-01	6.8776E-01	8.0080E-01
LPA (20:4)	0.1897	-0.6453	0.2502	0.2099	4.4958E-01	2.4826E-03	7.0240E-01	2.6245E-02
LPA (16:1)	0.2047	-0.3897	0.2708	0.2112	4.5086E-01	6.6834E-02	7.0240E-01	2.1028E-01
PAF 18(2)	0.1885	0.0359	0.2515	0.1979	4.5473E-01	8.5618E-01	7.0374E-01	9.3862E-01
5-HETrE/DGLA	-0.1791	-0.3653	0.2398	0.2001	4.5648E-01	6.9739E-02	7.0374E-01	2.1353E-01
SIP (18:0)	-0.2026	-0.3309	0.2729	0.2125	4.5900E-01	1.2150E-01	7.0395E-01	3.1273E-01
11,12-DiHETrE/11,12-EpETrE	-0.1747	-0.5564	0.2389	0.1898	4.6592E-01	3.8903E-03	7.0840E-01	3.1987E-02

Chapter III

Citrulline/Omithine	-0.1397	0.0813	0.1921	0.1632	4.6820E-01	6.1906E-01	7.0840E-01	8.2658E-01
15-HEPE/EPA	0.1792	0.0195	0.2470	0.2037	4.6918E-01	9.2371E-01	7.0840E-01	9.6611E-01
11,12-EpETrE	-0.1760	-0.2677	0.2437	0.1976	4.7147E-01	1.7742E-01	7.0840E-01	4.0089E-01
Sum HODEs	0.1935	0.0313	0.2711	0.2288	4.7657E-01	8.9146E-01	7.1245E-01	9.4578E-01
19,20-EpDPE	-0.1970	0.0900	0.2820	0.2432	4.8603E-01	7.1194E-01	7.2294E-01	8.6390E-01
LPS (22:6)	0.1301	0.2505	0.1880	0.1618	4.8991E-01	1.2367E-01	7.2507E-01	3.1288E-01
5-HETE	-0.1982	-0.8254	0.2898	0.2429	4.9511E-01	8.5618E-04	7.2578E-01	1.3868E-02
9-HOTrE	-0.1781	0.0723	0.2605	0.2158	4.9529E-01	7.3813E-01	7.2578E-01	8.6704E-01
10-HDoHE/DHA	0.2035	0.0037	0.2994	0.2389	4.9799E-01	9.8782E-01	7.2614E-01	9.9999E-01
8,12-iso- iPF2alpha-VI	-0.1938	-0.5456	0.2911	0.2396	5.0662E-01	2.4148E-02	7.2986E-01	1.2115E-01
9-HOTrE/ALA	-0.1703	0.1219	0.2571	0.2131	5.0893E-01	5.6814E-01	7.2986E-01	8.0080E-01
Cystathionine/Ho moCys	0.1917	-0.0006	0.2899	0.2234	5.0946E-01	9.9799E-01	7.2986E-01	9.9999E-01
Coriolic acid	0.1827	-0.0780	0.2769	0.2322	5.1041E-01	7.3721E-01	7.2986E-01	8.6704E-01
PGA2	0.1759	-0.2171	0.2707	0.2139	5.1684E-01	3.1164E-01	7.3277E-01	5.9131E-01
O-Acetyl-Ser	-0.1714	-0.0965	0.2641	0.1951	5.1740E-01	6.2149E-01	7.3277E-01	8.2658E-01
8-HDoHE/DHA	-0.1778	0.4788	0.2785	0.2445	5.2435E-01	5.2010E-02	7.3908E-01	1.7901E-01
SIP (18:2)	-0.1293	-0.8277	0.2134	0.1750	5.4569E-01	5.0710E-06	7.5879E-01	5.9617E-04
PGA2/AA	0.1429	0.1387	0.2374	0.1909	5.4809E-01	4.6848E-01	7.5879E-01	7.4155E-01
9-HpODE/LA	-0.1749	-0.2298	0.2905	0.2281	5.4815E-01	3.1527E-01	7.5879E-01	5.9333E-01
Gly-Gly	0.1477	-0.1352	0.2455	0.1962	5.4858E-01	4.9202E-01	7.5879E-01	7.6250E-01
9-KODE	-0.1546	-0.1131	0.2618	0.2256	5.5572E-01	6.1674E-01	7.6408E-01	8.2658E-01
17-HDoHE	0.1557	0.0590	0.2648	0.2143	5.5757E-01	7.8348E-01	7.6408E-01	8.9541E-01
13,14-dihydro-15- keto- PGF2alpha/AA	0.1575	0.1709	0.2734	0.2213	5.6538E-01	4.4117E-01	7.6857E-01	7.2092E-01
5-iPF2alpha- VI/AA	-0.1582	0.1911	0.2771	0.2334	5.6895E-01	4.1426E-01	7.6857E-01	6.9494E-01
Sum HETEs	0.1770	-0.5201	0.3160	0.2545	5.7619E-01	4.2600E-02	7.6857E-01	1.5957E-01
5-HEPE	-0.1426	-0.2166	0.2552	0.2221	5.7704E-01	3.3097E-01	7.6857E-01	6.1614E-01
cLPA (18:2)	0.1426	-0.2365	0.2554	0.2063	5.7751E-01	2.5337E-01	7.6857E-01	5.1368E-01
17-HDoHE/DHA	0.1700	0.1523	0.3048	0.2455	5.7790E-01	5.3596E-01	7.6857E-01	7.8150E-01
20-HETE	0.1613	-0.1242	0.2899	0.2300	5.7902E-01	5.9014E-01	7.6857E-01	8.1627E-01
14,15-DiHETE	0.1315	0.0047	0.2412	0.1899	5.8661E-01	9.8024E-01	7.7516E-01	9.9999E-01
12,13-DiHOME	-0.1077	-0.0545	0.1997	0.1666	5.9035E-01	7.4402E-01	7.7664E-01	8.6704E-01
AABA	-0.1563	0.1333	0.2942	0.2409	5.9589E-01	5.8092E-01	7.8045E-01	8.0729E-01
19,20- DiHDP/AA	0.1382	-0.1481	0.2637	0.2236	6.0115E-01	5.0869E-01	7.8387E-01	7.6993E-01
9-HODE/9- HpODE	0.1461	0.0247	0.2820	0.2201	6.0518E-01	9.1063E-01	7.8568E-01	9.5584E-01
Mead.Acid	-0.1415	-0.4768	0.2761	0.2311	6.0921E-01	4.0738E-02	7.8745E-01	1.5459E-01
LPG (16:1)	-0.1444	-0.4623	0.2944	0.2267	6.2458E-01	4.3126E-02	7.9302E-01	1.5957E-01
LPE (18:1)	-0.1244	-0.2768	0.2555	0.2033	6.2696E-01	1.7535E-01	7.9302E-01	3.9927E-01
cLPA (14:0)	-0.0974	-0.3646	0.2006	0.1569	6.2790E-01	2.1385E-02	7.9302E-01	1.1509E-01
LPI (20:4)	0.1272	-0.2582	0.2636	0.2141	6.2999E-01	2.2961E-01	7.9302E-01	4.7197E-01
8-HDoHE	-0.1119	0.2168	0.2325	0.1953	6.3096E-01	2.6868E-01	7.9302E-01	5.3376E-01
AdA	-0.1387	-0.5019	0.2900	0.2359	6.3321E-01	3.4931E-02	7.9302E-01	1.4855E-01
13,14-dihydro-15- keto-PGF2alpha	0.1266	-0.1090	0.2670	0.2224	6.3611E-01	6.2485E-01	7.9302E-01	8.2658E-01
1-Met-His	-0.1383	-0.3672	0.2928	0.2312	6.3742E-01	1.1421E-01	7.9302E-01	2.9917E-01
cLPA (18:1)	0.1203	-0.2565	0.2549	0.2059	6.3763E-01	2.1475E-01	7.9302E-01	4.6062E-01
SIP (18:1)	-0.1010	-0.6801	0.2198	0.1884	6.4659E-01	4.1519E-04	8.0080E-01	7.6811E-03
Glucose	0.1182	-0.0775	0.2654	0.2308	6.5690E-01	7.3753E-01	8.1016E-01	8.6704E-01
Cys/Cystathionine	-0.1347	0.0522	0.3053	0.2328	6.5962E-01	8.2296E-01	8.1016E-01	9.1838E-01
9-HpODE	-0.1037	0.0012	0.2567	0.2073	6.6890E-01	9.9541E-01	8.4017E-01	9.9999E-01
9-HEPE	0.0857	0.0699	0.2252	0.1827	7.0420E-01	7.0254E-01	8.5448E-01	8.6175E-01
ALA	-0.0779	0.0233	0.2049	0.1571	7.0437E-01	8.8229E-01	8.5448E-01	9.4347E-01
LPS (20:4)	-0.0803	-0.2785	0.2143	0.1794	7.0860E-01	1.2263E-01	8.5526E-01	3.1288E-01
OA	-0.0977	-0.6471	0.2648	0.2373	7.1267E-01	7.1056E-03	8.5526E-01	4.8829E-02
EA	-0.0842	0.3781	0.2291	0.1823	7.1368E-01	3.9737E-02	8.5526E-01	1.5459E-01
OH-Lys/Lys	-0.0926	-0.1774	0.2684	0.2205	7.3057E-01	4.2219E-01	8.6348E-01	7.0207E-01
AA	0.1029	-0.4610	0.3005	0.2454	7.3258E-01	6.2155E-02	8.6348E-01	2.0217E-01
LPG (16:0)	-0.0949	-0.1386	0.2774	0.2229	7.3280E-01	5.3511E-01	8.6348E-01	7.8150E-01
DEA	-0.1023	0.4374	0.3036	0.2326	7.3683E-01	6.1962E-02	8.6348E-01	2.0217E-01
LPG (14:0)	-0.0601	-0.4646	0.1792	0.1443	7.3770E-01	1.5603E-03	8.6348E-01	2.0396E-02
ETE	0.0986	-0.5190	0.2977	0.2449	7.4099E-01	3.5680E-02	8.6348E-01	1.4855E-01
11beta- PGF2alpha/AA	-0.0792	0.2872	0.2396	0.1895	7.4140E-01	1.3190E-01	8.6348E-01	3.2645E-01
LPI (22:6)	0.0865	-0.2624	0.2645	0.2332	7.4419E-01	2.6221E-01	8.6348E-01	5.2442E-01
Sum iPs	-0.0818	0.0993	0.2560	0.2227	7.4997E-01	6.5629E-01	8.6348E-01	8.5202E-01
7-HDoHE/DHA	-0.0927	0.2274	0.2934	0.2476	7.5249E-01	3.5980E-01	8.6348E-01	6.3773E-01
O-PO3-EA	0.0894	-0.1885	0.2832	0.2380	7.5263E-01	4.2972E-01	8.6348E-01	7.1060E-01

Diagnosis of Late-Onset Sepsis

LPE (18:3)	-0.0765	-0.1316	0.2514	0.1953	7.6136E-01	5.0139E-01	8.7012E-01	7.6501E-01
cLPA (20:4)	0.0784	-0.1979	0.2627	0.2118	7.6583E-01	3.5158E-01	8.7187E-01	6.3456E-01
17,18-DiHETE	-0.0737	0.0317	0.2578	0.2129	7.7548E-01	8.8174E-01	8.7219E-01	9.4347E-01
TUDCA	0.0660	0.1847	0.2333	0.2084	7.7757E-01	3.7689E-01	8.7219E-01	6.5239E-01
LPE (22:5)	-0.0831	-0.3264	0.2955	0.2346	7.7905E-01	1.6610E-01	8.7219E-01	3.8410E-01
Phe	-0.0758	-0.1353	0.2729	0.2154	7.8150E-01	5.3091E-01	8.7219E-01	7.8150E-01
DGLA	-0.0795	-0.1486	0.2882	0.2375	7.8312E-01	5.3248E-01	8.7219E-01	7.8150E-01
FA (16:0)	-0.0804	-0.3276	0.2923	0.2456	7.8379E-01	1.8423E-01	8.7219E-01	4.0761E-01
LA	0.0551	0.2563	0.2122	0.1694	7.9570E-01	1.3234E-01	8.8212E-01	3.2645E-01
LPE (16:1)	-0.0693	-0.4590	0.2721	0.2120	7.9933E-01	3.2081E-02	8.8284E-01	1.4173E-01
5-OH-Trp	-0.0723	-0.6208	0.2909	0.2398	8.0415E-01	1.0525E-02	8.8486E-01	6.6286E-02
EPA	0.0393	0.0871	0.1658	0.1293	8.1316E-01	5.0130E-01	8.9146E-01	7.6501E-01
beta-Ala	-0.0599	-0.1301	0.2684	0.2044	8.2363E-01	5.2548E-01	8.9343E-01	7.8150E-01
LPS (16:0)	-0.0654	0.2322	0.2933	0.2312	8.2384E-01	3.1671E-01	8.9343E-01	5.9333E-01
LPA (22:4)	-0.0683	-0.5851	0.3082	0.2557	8.2506E-01	2.3432E-02	8.9343E-01	1.1959E-01
2,3-dinor-8-iso-PGF2alpha	-0.0680	-0.0954	0.3104	0.2581	8.2703E-01	7.1213E-01	8.9343E-01	8.6390E-01
8-iso-PGF3alpha/DGLA	-0.0476	0.0736	0.2287	0.1909	8.3560E-01	7.0035E-01	8.9812E-01	8.6175E-01
LPG (22:6)	-0.0355	0.0767	0.1746	0.1373	8.3911E-01	5.7693E-01	8.9812E-01	8.0553E-01
7-HDoHE	-0.0475	0.0951	0.2380	0.1983	8.4220E-01	6.3224E-01	8.9812E-01	8.3175E-01
5,6-DiHETrE	-0.0487	-0.8655	0.2461	0.2022	8.4351E-01	3.2230E-05	8.9812E-01	1.7083E-03
DHA	0.0410	-0.0439	0.2268	0.1855	8.5697E-01	8.1308E-01	9.0918E-01	9.1605E-01
Sum DiHETEs	0.0458	-0.0798	0.2646	0.2090	8.6283E-01	7.0326E-01	9.1213E-01	8.6175E-01
LPG (18:0)	-0.0400	0.0483	0.2699	0.2049	8.8251E-01	8.1392E-01	9.2937E-01	9.1605E-01
w3FA/w6FA	0.0238	0.3132	0.1647	0.1354	8.8542E-01	2.2024E-02	9.2937E-01	1.1627E-01
5-iPF2alpha-VI	-0.0265	-0.1864	0.2730	0.2183	9.2293E-01	3.9464E-01	9.6263E-01	6.7523E-01
FA (18:0)	0.0272	-0.0901	0.2837	0.2370	9.2372E-01	7.0454E-01	9.6263E-01	8.6175E-01
13-HDoHE	0.0223	0.2585	0.2428	0.1987	9.2686E-01	1.9512E-01	9.6263E-01	4.2157E-01
Met-SO2	0.0168	-0.3804	0.2274	0.1716	9.4132E-01	2.8096E-02	9.7424E-01	1.3276E-01
S1P (16:1)	-0.0102	-0.6470	0.1848	0.1635	9.5609E-01	1.1520E-04	9.8266E-01	3.0999E-03
20-HETE/AA	-0.0146	0.3196	0.2641	0.2134	9.5610E-01	1.3639E-01	9.8266E-01	3.2941E-01
9-HEPE/EPA	-0.0123	-0.0394	0.2762	0.2252	9.6447E-01	8.6145E-01	9.8548E-01	9.4092E-01
16-HDoHE/DHA	-0.0123	0.3334	0.2854	0.2443	9.6558E-01	1.7427E-01	9.8548E-01	3.9927E-01
Clupanodonic acid	-0.0092	-0.0527	0.2355	0.1908	9.6884E-01	7.8279E-01	9.8548E-01	8.9541E-01
13-HDoHE/DHA	0.0074	0.4895	0.2888	0.2452	9.7972E-01	4.7592E-02	9.9314E-01	1.6784E-01
19,20-DiHDPA	0.0054	-0.0766	0.2913	0.2287	9.8528E-01	7.3828E-01	9.9487E-01	8.6704E-01
16-HDoHE	-0.0027	0.1438	0.2289	0.1904	9.9059E-01	4.5115E-01	9.9487E-01	7.2346E-01
2,3-dinor-8-iso-PGF2alpha/AA	0.0025	0.2304	0.2999	0.2592	9.9347E-01	3.7541E-01	9.9487E-01	6.5239E-01
5-aminolevulinic acid	-0.0019	0.0129	0.2928	0.2263	9.9487E-01	9.5470E-01	9.9487E-01	9.8808E-01

Table S11: Logistic regression results of the "C_SINS" model comparing control with systemic inflammation-no sepsis in the single time point dataset

Metabolite	Category	Estimate	Standard Error	z-value	p-value	Adjusted p-value
LPS (18:0)	Lysophospholipid	3.6885	1.1570	3.1879	1.4333E-03	2.3753E-01
Ser	Amine	-3.6882	1.2387	-2.9776	2.9055E-03	2.3753E-01
Thr	Amine	-4.2410	1.4796	-2.8663	4.1527E-03	2.3753E-01
His	Amine	-3.7968	1.3669	-2.7776	5.4755E-03	2.3753E-01
Ornithine	Amine	-3.6618	1.3772	-2.6589	7.8392E-03	2.3753E-01
Lys	Amine	-2.9695	1.1224	-2.6458	8.1497E-03	2.3753E-01
Cortisol	Steroid Hormone	1.5693	0.5997	2.6168	8.8763E-03	2.3753E-01
Trp	Amine	-11.0103	4.2531	-2.5888	9.6322E-03	2.3753E-01
Gly	Amine	-3.7189	1.4481	-2.5681	1.0225E-02	2.3753E-01
cLPA (20:4)	Lysophospholipid	-2.0055	0.7884	-2.5438	1.0966E-02	2.3753E-01
S1P (18:2)	Lysophospholipid	-4.1930	1.6575	-2.5297	1.1415E-02	2.3753E-01
Asn	Amine	-2.8495	1.1364	-2.5075	1.2158E-02	2.3753E-01
Met	Amine	-2.7373	1.1203	-2.4433	1.4553E-02	2.3753E-01
LPS (18:2)	Lysophospholipid	1.7778	0.7292	2.4381	1.4766E-02	2.3753E-01
4-OH-Pro	Amine	-3.0991	1.2765	-2.4278	1.5190E-02	2.3753E-01
LPS (18:1)	Lysophospholipid	1.6731	0.6991	2.3932	1.6701E-02	2.3753E-01
Sum SBA	Bile Acid	-2.3664	1.0019	-2.3619	1.8180E-02	2.3753E-01
5-HETE/AA	Oxylipin	-2.6759	1.1334	-2.3610	1.8226E-02	2.3753E-01
LPE (22:4)	Lysophospholipid	-1.7102	0.7259	-2.3560	1.8475E-02	2.3753E-01
S1P (16:1)	Lysophospholipid	-2.8304	1.2051	-2.3488	1.8835E-02	2.3753E-01
LCA	Bile Acid	-3.0814	1.3234	-2.3285	1.9887E-02	2.3753E-01
OH-Lys	Amine	-2.8683	1.2370	-2.3187	2.0414E-02	2.3753E-01
cLPA (18:2)	Lysophospholipid	-1.3306	0.5754	-2.3124	2.0758E-02	2.3753E-01
Arg	Amine	-1.5481	0.6744	-2.2956	2.1697E-02	2.3753E-01
AAA	Amine	-2.4401	1.0652	-2.2907	2.1980E-02	2.3753E-01
Gln	Amine	-1.6820	0.7399	-2.2733	2.3009E-02	2.3753E-01

Chapter III

8,9-DIHETrE	Oxylipin	-1.2161	0.5375	-2.2623	2.3680E-02	2.3753E-01
TLCA-3S	Bile Acid	-0.7381	0.3264	-2.2612	2.3747E-02	2.3753E-01
g-Glu-Gln	Amine	-1.1687	0.5172	-2.2596	2.3847E-02	2.3753E-01
Saccharopine	Amine	-1.4019	0.6223	-2.2529	2.4267E-02	2.3753E-01
PGF1alpha	Oxylipin	-1.2115	0.5401	-2.2433	2.4877E-02	2.3753E-01
Sum DIHETrEs	Oxylipin	-1.4770	0.6651	-2.2206	2.6378E-02	2.4400E-01
14-HDoHE	Oxylipin	0.7285	0.3300	2.2075	2.7277E-02	2.4466E-01
Val	Amine	-2.9191	1.3401	-2.1783	2.9386E-02	2.5482E-01
14-HDoHE/DHA	Oxylipin	0.8199	0.3781	2.1684	3.0131E-02	2.5482E-01
Cys	Amine	-1.9348	0.9013	-2.1467	3.1819E-02	2.6162E-01
BCAA	Amine	-2.8576	1.3425	-2.1285	3.3298E-02	2.6638E-01
Sum HEPEs	Oxylipin	0.7573	0.3627	2.0880	3.6794E-02	2.8255E-01
5,6-DIHETrE	Oxylipin	-0.9584	0.4653	-2.0597	3.9428E-02	2.8255E-01
Sum BA	Bile Acid	-0.4265	0.2073	-2.0581	3.9583E-02	2.8255E-01
Tyr	Amine	-1.3170	0.6429	-2.0484	4.0524E-02	2.8255E-01
18-HEPE	Oxylipin	0.8627	0.4219	2.0446	4.0891E-02	2.8255E-01
Leu	Amine	-3.0740	1.5055	-2.0418	4.1169E-02	2.8255E-01
Sarcosine	Amine	-1.1006	0.5417	-2.0316	4.2192E-02	2.8255E-01
Sum HDoHEs	Oxylipin	0.7459	0.3685	2.0241	4.2955E-02	2.8255E-01
LPI (18:0)	Lysophospholipid	2.1816	1.0947	1.9929	4.6276E-02	2.9777E-01
S1P (18:1)	Lysophospholipid	-2.1950	1.1071	-1.9827	4.7400E-02	2.9852E-01
Ile	Amine	-2.3729	1.2138	-1.9550	5.0578E-02	3.1062E-01
LPE (20:3)	Lysophospholipid	-1.5938	0.8182	-1.9480	5.1420E-02	3.1062E-01
12-HEPE	Oxylipin	0.6009	0.3127	1.9217	5.4648E-02	3.2281E-01
Sum OG	Endocannabinoid	-1.1647	0.6122	-1.9023	5.7128E-02	3.2281E-01
Phe/Tyr	Amine	1.3331	0.7054	1.8900	5.8762E-02	3.2281E-01
LPS (16:0)	Lysophospholipid	4.5929	2.4305	1.8897	5.8798E-02	3.2281E-01
GCDCA	Bile Acid	-0.3787	0.2005	-1.8890	5.8892E-02	3.2281E-01
5-HETE	Oxylipin	-1.2255	0.6544	-1.8726	6.1123E-02	3.2895E-01
O-Acetyl-Ser	Amine	-1.4629	0.7890	-1.8541	6.3721E-02	3.3349E-01
Sum LG	Endocannabinoid	-0.9051	0.4905	-1.8452	6.5008E-02	3.3349E-01
ADMA	Amine	-2.0401	1.1106	-1.8369	6.6218E-02	3.3349E-01
5-KETE/5-HETE	Oxylipin	1.3402	0.7303	1.8352	6.6473E-02	3.3349E-01
Arg/ADMA	Amine	-1.4161	0.7871	-1.7991	7.2001E-02	3.5023E-01
S-Methyl-Cys	Amine	-1.9398	1.0793	-1.7973	7.2288E-02	3.5023E-01
Tau	Amine	1.2502	0.6987	1.7893	7.3570E-02	3.5023E-01
11-HDoHE	Oxylipin	0.6090	0.3415	1.7833	7.4542E-02	3.5023E-01
HomoCys	Amine	-1.2900	0.7265	-1.7756	7.5800E-02	3.5075E-01
LPG (20:3)	Lysophospholipid	-2.0566	1.1634	-1.7677	7.7116E-02	3.5118E-01
Sum AG	Endocannabinoid	-0.7822	0.4463	-1.7527	7.9657E-02	3.5579E-01
LPS (20:4)	Lysophospholipid	1.3044	0.7464	1.7476	8.0534E-02	3.5579E-01
Gln/Glu	Amine	-0.8021	0.4638	-1.7295	8.3728E-02	3.6446E-01
11-HDoHE/DHA	Oxylipin	0.7180	0.4201	1.7092	8.7410E-02	3.7145E-01
8-HETrE/DGLA	Oxylipin	0.7234	0.4238	1.7069	8.7843E-02	3.7145E-01
9-HEPE	Oxylipin	0.7467	0.4416	1.6908	9.0877E-02	3.7738E-01
14,15-DIHETrE	Oxylipin	-1.0621	0.6300	-1.6860	9.1795E-02	3.7738E-01
10-HDoHE	Oxylipin	0.6445	0.3853	1.6727	9.4384E-02	3.7770E-01
11beta-PGF2alpha	Oxylipin	-0.7488	0.4477	-1.6725	9.4426E-02	3.7770E-01
GCA	Bile Acid	-0.3085	0.1857	-1.6612	9.6665E-02	3.7837E-01
5-HT/Trp	Amine	0.4423	0.2683	1.6485	9.9242E-02	3.7837E-01
LPS (22:6)	Lysophospholipid	1.0478	0.6356	1.6485	9.9252E-02	3.7837E-01
LPE (20:4)	Lysophospholipid	-1.5447	0.9383	-1.6463	9.9705E-02	3.7837E-01
Citrulline/Ornithine	Amine	1.1890	0.7259	1.6380	1.0143E-01	3.8005E-01
11,12-DIHETrE	Oxylipin	-0.8386	0.5208	-1.6102	1.0737E-01	3.9725E-01
10-HDoHE/DHA	Oxylipin	0.7826	0.4882	1.6031	1.0892E-01	3.9803E-01
12-HETE/AA	Oxylipin	0.6034	0.3842	1.5706	1.1627E-01	4.1857E-01
15-HEPE	Oxylipin	0.7532	0.4810	1.5659	1.1737E-01	4.1857E-01
LPE (22:6)	Lysophospholipid	-1.6799	1.0868	-1.5457	1.2218E-01	4.2568E-01
Met-SO2	Amine	-1.2866	0.8328	-1.5450	1.2234E-01	4.2568E-01
12-HEPE/EPA	Oxylipin	0.5545	0.3602	1.5395	1.2368E-01	4.2568E-01
eLPA (18:1)	Lysophospholipid	-0.7889	0.5277	-1.4950	1.3490E-01	4.5898E-01
11beta-PGF2alpha/AA	Oxylipin	-0.5383	0.3642	-1.4780	1.3942E-01	4.6895E-01
LPG (20:4)	Lysophospholipid	-1.3144	0.8931	-1.4717	1.4110E-01	4.6928E-01
18-HEPE/EPA	Oxylipin	0.7488	0.5134	1.4586	1.4467E-01	4.7266E-01
Sum PGs	Oxylipin	-0.4300	0.2960	-1.4526	1.4633E-01	4.7266E-01
Ala	Amine	-1.9449	1.3408	-1.4505	1.4691E-01	4.7266E-01
12-HETE	Oxylipin	0.4753	0.3323	1.4305	1.5257E-01	4.8560E-01
4-OH-Pro/Pro	Amine	-1.4828	1.0438	-1.4205	1.5546E-01	4.8606E-01
20-HDoHE	Oxylipin	0.6516	0.4606	1.4147	1.5716E-01	4.8606E-01
17,18-DIHETE	Oxylipin	-0.5240	0.3708	-1.4130	1.5764E-01	4.8606E-01
PGF1alpha/DGLA	Oxylipin	-0.4179	0.2992	-1.3969	1.6244E-01	4.9454E-01
CA	Bile Acid	0.3599	0.2584	1.3926	1.6373E-01	4.9454E-01
LPI (16:0)	Lysophospholipid	1.2481	0.9075	1.3754	1.6901E-01	5.0533E-01
5-HEPE/EPA	Oxylipin	-0.8711	0.6392	-1.3629	1.7291E-01	5.1182E-01

Diagnosis of Late-Onset Sepsis

Homoserine	Amine	-1.3830	1.0247	-1.3496	1.7713E-01	5.1911E-01
LPS (22:4)	Lysophospholipid	1.1171	0.8483	1.3169	1.8788E-01	5.4252E-01
LPE (18:3)	Lysophospholipid	0.5192	0.3966	1.3090	1.9053E-01	5.4252E-01
LPE (16:0)	Lysophospholipid	1.0753	0.8248	1.3038	1.9229E-01	5.4252E-01
8-HETE	Oxylipin	0.5235	0.4017	1.3034	1.9245E-01	5.4252E-01
LPG (14:0)	Lysophospholipid	-1.0556	0.8149	-1.2953	1.9521E-01	5.4511E-01
Gly-Pro	Amine	-0.7061	0.5490	-1.2861	1.9839E-01	5.4883E-01
Citrulline	Amine	-0.9005	0.7103	-1.2678	2.0489E-01	5.6154E-01
Trimethyl-Lys	Amine	-1.5818	1.2639	-1.2515	2.1075E-01	5.7231E-01
g-Glu-Ala	Amine	-0.5564	0.4476	-1.2433	2.1377E-01	5.7273E-01
EPA	Fatty acid	0.5740	0.4627	1.2406	2.1477E-01	5.7273E-01
BCAA/Tyr	Amine	0.8319	0.6743	1.2337	2.1730E-01	5.7429E-01
GLA	Fatty acid	-1.1811	0.9652	-1.2237	2.2107E-01	5.7908E-01
Kyn	Amine	-0.6575	0.5453	-1.2056	2.2797E-01	5.9191E-01
17-HDoHE	Oxylipin	0.4600	0.3854	1.1936	2.3263E-01	5.9285E-01
LPE (22:5)	Lysophospholipid	-0.7814	0.6555	-1.1920	2.3328E-01	5.9285E-01
LPE (18:2)	Lysophospholipid	-0.7613	0.6432	-1.1837	2.3654E-01	5.9285E-01
LPI (22:6)	Lysophospholipid	-1.2311	1.0453	-1.1778	2.3889E-01	5.9285E-01
TCA	Bile Acid	-0.3309	0.2838	-1.1663	2.4349E-01	5.9285E-01
LPE (20:5)	Lysophospholipid	-1.0070	0.8663	-1.1624	2.4507E-01	5.9285E-01
LPI (18:1)	Lysophospholipid	1.3834	1.1901	1.1624	2.4507E-01	5.9285E-01
12,13-DiHOME/12,13-EpOME	Oxylipin	-0.5448	0.4696	-1.1601	2.4600E-01	5.9285E-01
Pro	Amine	-1.3211	1.1414	-1.1574	2.4709E-01	5.9285E-01
8,12-iso-iPF2alpha-VI/AA	Oxylipin	-0.8733	0.7582	-1.1517	2.4943E-01	5.9285E-01
LPG (18:2)	Lysophospholipid	-0.7774	0.6777	-1.1472	2.5132E-01	5.9285E-01
19,20-EpDPE/DHA	Oxylipin	-0.6529	0.5704	-1.1446	2.5236E-01	5.9285E-01
Sum HETrEs	Oxylipin	0.4791	0.4231	1.1323	2.5750E-01	6.0015E-01
20-HDoHE/DHA	Oxylipin	0.5969	0.5340	1.1179	2.6362E-01	6.0864E-01
SDMA	Amine	-0.9707	0.8748	-1.1097	2.6714E-01	6.0864E-01
Phe	Amine	-1.2993	1.1726	-1.1081	2.6782E-01	6.0864E-01
17-HDoHE/DHA	Oxylipin	0.6183	0.5608	1.1025	2.7025E-01	6.0864E-01
ALA	Fatty acid	0.6379	0.5800	1.0998	2.7142E-01	6.0864E-01
LPG (18:1)	Lysophospholipid	-1.3018	1.1907	-1.0934	2.7423E-01	6.1031E-01
LPI (20:4)	Lysophospholipid	-1.1017	1.0140	-1.0866	2.7724E-01	6.1240E-01
LPG (16:1)	Lysophospholipid	-0.7584	0.7019	-1.0805	2.7994E-01	6.1379E-01
15-HETE/DGLA	Oxylipin	0.4438	0.4256	1.0427	2.9708E-01	6.4659E-01
9-HODE/9-HpODE	Oxylipin	0.6071	0.6049	1.0036	3.1557E-01	6.7900E-01
Sum DiHETEs	Oxylipin	-0.3910	0.3923	-0.9967	3.1890E-01	6.7900E-01
LPA (20:4)	Lysophospholipid	-0.7857	0.7899	-0.9947	3.1990E-01	6.7900E-01
cLPA (18:0)	Lysophospholipid	-0.6610	0.6680	-0.9896	3.2237E-01	6.7900E-01
FA (18:0)	Fatty acid	0.6727	0.6813	0.9874	3.2344E-01	6.7900E-01
cLPA (16:1)	Lysophospholipid	-0.8328	0.8604	-0.9679	3.3307E-01	6.8885E-01
w3FA/w6FA	Fatty acid	0.8111	0.8396	0.9660	3.3406E-01	6.8885E-01
LPA (18:2)	Lysophospholipid	-0.6894	0.7152	-0.9639	3.3512E-01	6.8885E-01
5-aminolevulinic acid	Amine	0.6232	0.6653	0.9367	3.4891E-01	7.0137E-01
SIP (18:0)	Lysophospholipid	-0.5209	0.5582	-0.9332	3.5072E-01	7.0137E-01
9-HEPE/EPA	Oxylipin	0.5822	0.6241	0.9329	3.5086E-01	7.0137E-01
beta-Ala	Amine	-0.9077	0.9759	-0.9301	3.5232E-01	7.0137E-01
13-HDoHE	Oxylipin	0.4382	0.4748	0.9231	3.5597E-01	7.0137E-01
11-HETE/AA	Oxylipin	-0.5476	0.5955	-0.9196	3.5781E-01	7.0137E-01
Kyn/Trp	Amine	0.5713	0.6239	0.9158	3.5978E-01	7.0137E-01
LPG (22:4)	Lysophospholipid	-0.7421	0.8126	-0.9133	3.6107E-01	7.0137E-01
LPI (22:4)	Lysophospholipid	-0.8147	0.8947	-0.9106	3.6253E-01	7.0137E-01
LPE (16:1)	Lysophospholipid	-0.6190	0.6837	-0.9053	3.6531E-01	7.0215E-01
5-OH-Trp	Amine	0.7437	0.8267	0.8995	3.6836E-01	7.0345E-01
PAF 18(2)	PAF	-0.2535	0.2837	-0.8938	3.7145E-01	7.0480E-01
5-HT	Amine	0.2213	0.2510	0.8815	3.7802E-01	7.1270E-01
8,12-iso-iPF2alpha-VI	Oxylipin	-0.5426	0.6203	-0.8747	3.8172E-01	7.1512E-01
Anserine	Amine	-0.3684	0.4292	-0.8585	3.9062E-01	7.2703E-01
Sphingosine 18.1	Lysophospholipid	-0.4602	0.5427	-0.8480	3.9644E-01	7.2703E-01
Cystathionine	Amine	-0.2972	0.3510	-0.8466	3.9720E-01	7.2703E-01
11,12-EpETrE/AA	Oxylipin	-0.5081	0.6010	-0.8454	3.9790E-01	7.2703E-01
Ada	Fatty acid	-0.4075	0.4857	-0.8391	4.0142E-01	7.2896E-01
LPA (22:4)	Lysophospholipid	-0.4784	0.5742	-0.8332	4.0473E-01	7.3050E-01
11,12-DiHETrE/11,12-EpETrE	Oxylipin	-0.3347	0.4069	-0.8225	4.1077E-01	7.3690E-01
OH-Lys/Lys	Amine	0.7081	0.8744	0.8098	4.1804E-01	7.4542E-01
3-Methoxy-tyramine	Amine	1.0141	1.3043	0.7775	4.3687E-01	7.7433E-01
9-HOTrE	Oxylipin	0.3315	0.4297	0.7715	4.4042E-01	7.7598E-01
O-PO3-EA	Amine	0.3620	0.4760	0.7605	4.4695E-01	7.8283E-01
LPE (14:0)	Lysophospholipid	-0.4563	0.6080	-0.7505	4.5293E-01	7.8863E-01
Sum KETEs	Oxylipin	0.2241	0.3005	0.7457	4.5587E-01	7.8910E-01
LPG (18:0)	Lysophospholipid	0.5591	0.7620	0.7338	4.6307E-01	7.9691E-01
13,14-dihydro-15-keto-PGF2alpha/AA	Oxylipin	-0.2932	0.4053	-0.7235	4.6936E-01	8.0138E-01
BCAA/AAA	Amine	0.7459	1.0350	0.7207	4.7108E-01	8.0138E-01

Chapter III

DEA	Endocannabinoid	0.3300	0.4638	0.7114	4.7683E-01	8.0652E-01
11,12-EpETrE	Oxylipin	-0.3616	0.5286	-0.6841	4.9391E-01	8.2344E-01
3-AIBA	Amine	0.2375	0.3478	0.6828	4.9476E-01	8.2344E-01
12,13-DIHOME	Oxylipin	-0.2510	0.3715	-0.6757	4.9924E-01	8.2344E-01
9-HpODE/LA	Oxylipin	-0.3327	0.4952	-0.6719	5.0162E-01	8.2344E-01
11-HETE	Oxylipin	-0.3068	0.4629	-0.6628	5.0747E-01	8.2344E-01
LPA (20:5)	Lysophospholipid	0.4127	0.6246	0.6607	5.0878E-01	8.2344E-01
9-HpODE	Oxylipin	-0.3325	0.5033	-0.6606	5.0887E-01	8.2344E-01
Sum PBA	Bile Acid	-0.1330	0.2014	-0.6603	5.0908E-01	8.2344E-01
EA	Amine	0.5153	0.7861	0.6555	5.1212E-01	8.2384E-01
Coriolic acid	Oxylipin	0.2795	0.4354	0.6419	5.2095E-01	8.3260E-01
5-IPF2alpha-VI/AA	Oxylipin	-0.4410	0.6908	-0.6384	5.2319E-01	8.3260E-01
cLPA (14:0)	Lysophospholipid	-0.4468	0.7198	-0.6208	5.3475E-01	8.4644E-01
3-Methoxy-tyrosine	Amine	-0.4059	0.6694	-0.6063	5.4429E-01	8.5611E-01
15-HETrE	Oxylipin	0.2468	0.4093	0.6028	5.4664E-01	8.5611E-01
Carnosine	Amine	0.2897	0.5014	0.5777	5.6344E-01	8.7506E-01
Glu	Amine	-0.6530	1.1338	-0.5759	5.6465E-01	8.7506E-01
LPE (18:0)	Lysophospholipid	0.4724	0.8321	0.5677	5.7027E-01	8.7717E-01
13,14-dihydro-15-keto-PGF2alpha	Oxylipin	-0.2271	0.4037	-0.5626	5.7369E-01	8.7717E-01
19,20-DiHDDPA	Oxylipin	-0.2380	0.4243	-0.5608	5.7491E-01	8.7717E-01
Sum iPs	Oxylipin	0.1213	0.2214	0.5482	5.8358E-01	8.8585E-01
PAF 16(0)	PAF	-0.2546	0.4706	-0.5410	5.8847E-01	8.8872E-01
LPG 16(0:0)	Lysophospholipid	-0.5632	1.0620	-0.5303	5.9593E-01	8.9109E-01
19,20-EpDPE	Oxylipin	-0.2525	0.4763	-0.5301	5.9606E-01	8.9109E-01
PGA2/AA	Oxylipin	-0.2602	0.4993	-0.5211	6.0230E-01	8.9588E-01
12-KETE/12-HETE	Oxylipin	-0.1546	0.2997	-0.5160	6.0589E-01	8.9671E-01
13-HDoHE/DHA	Oxylipin	0.2822	0.5531	0.5103	6.0985E-01	8.9792E-01
HCA	Bile Acid	-0.0950	0.1880	-0.5053	6.1337E-01	8.9792E-01
15-HEPE/EPA	Oxylipin	0.2765	0.5556	0.4977	6.1867E-01	8.9792E-01
Arg/Lys	Amine	-0.3757	0.7564	-0.4967	6.1942E-01	8.9792E-01
delta-17,6-keto-PGF1alpha	Oxylipin	0.1027	0.2111	0.4863	6.2677E-01	8.9792E-01
DHA	Fatty acid	0.2184	0.4526	0.4825	6.2947E-01	8.9792E-01
Glu/GABA	Amine	-0.3739	0.7770	-0.4812	6.3035E-01	8.9792E-01
LPA (22:5)	Lysophospholipid	-0.3061	0.6371	-0.4804	6.3097E-01	8.9792E-01
DGLA	Fatty acid	-0.2064	0.4364	-0.4731	6.3618E-01	9.0043E-01
16-HDoHE/DHA	Oxylipin	-0.2744	0.5846	-0.4693	6.3882E-01	9.0043E-01
delta-17,6-keto-PGF1alpha/EPA	Oxylipin	0.1017	0.2214	0.4592	6.4611E-01	9.0492E-01
Sphinganine 18.0	Lysophospholipid	-0.2603	0.5748	-0.4529	6.5062E-01	9.0492E-01
Cys/Cystathionine	Amine	-0.1417	0.3134	-0.4521	6.5118E-01	9.0492E-01
Sum HODEs	Oxylipin	0.1945	0.4450	0.4371	6.6207E-01	9.1161E-01
Met-SO	Amine	0.4543	1.0409	0.4365	6.6250E-01	9.1161E-01
Glutathione	Amine	0.1832	0.4233	0.4327	6.6523E-01	9.1161E-01
LPI (18:2)	Lysophospholipid	-0.3165	0.7451	-0.4247	6.7105E-01	9.1534E-01
Cystathionine/HomoCys	Amine	0.1251	0.3043	0.4111	6.8102E-01	9.2049E-01
8-HDoHE/DHA	Oxylipin	-0.2310	0.5619	-0.4111	6.8104E-01	9.2049E-01
Mead.Acid	Fatty acid	0.1483	0.3705	0.4003	6.8896E-01	9.2201E-01
TUDCA	Bile Acid	-0.1171	0.2962	-0.3953	6.9264E-01	9.2201E-01
THDCA	Bile Acid	-0.1258	0.3294	-0.3818	7.0261E-01	9.2201E-01
LPE (18:1)	Lysophospholipid	0.2705	0.7234	0.3740	7.0841E-01	9.2201E-01
TXB3	Oxylipin	0.0973	0.2664	0.3652	7.1500E-01	9.2201E-01
LPA (20:3)	Lysophospholipid	-0.2440	0.6712	-0.3635	7.1626E-01	9.2201E-01
7-HDoHE	Oxylipin	0.1559	0.4295	0.3630	7.1662E-01	9.2201E-01
LPG (22:6)	Lysophospholipid	-0.3218	0.8925	-0.3605	7.1845E-01	9.2201E-01
DHEA	Endocannabinoid	0.2488	0.6915	0.3598	7.1903E-01	9.2201E-01
LPA (14:0)	Lysophospholipid	-0.2150	0.6031	-0.3565	7.2145E-01	9.2201E-01
TXB3/EPA	Oxylipin	-0.0927	0.2667	-0.3476	7.2813E-01	9.2201E-01
5-IPF2alpha-VI	Oxylipin	-0.2168	0.6251	-0.3468	7.2873E-01	9.2201E-01
PGE1	Oxylipin	-0.1002	0.2908	-0.3445	7.3048E-01	9.2201E-01
12,13-EpOME	Oxylipin	0.1555	0.4517	0.3443	7.3060E-01	9.2201E-01
LPG (18:3)	Lysophospholipid	0.2434	0.7083	0.3437	7.3109E-01	9.2201E-01
12,13-EpOME/LA	Oxylipin	0.1636	0.4778	0.3425	7.3200E-01	9.2201E-01
LPA (16:1)	Lysophospholipid	-0.1569	0.4774	-0.3287	7.4239E-01	9.3113E-01
Sum TxS	Oxylipin	0.0849	0.2742	0.3095	7.5693E-01	9.4537E-01
5-HETrE	Oxylipin	-0.1193	0.3997	-0.2986	7.6528E-01	9.5178E-01
LPI (16:1)	Lysophospholipid	-0.1763	0.6217	-0.2836	7.7668E-01	9.6053E-01
OA	Fatty acid	-0.4460	1.5879	-0.2809	7.7881E-01	9.6053E-01
DPA	Fatty acid	-0.1069	0.3966	-0.2695	7.8755E-01	9.6728E-01
LPA (22:6)	Lysophospholipid	-0.1712	0.6746	-0.2538	7.9964E-01	9.7762E-01
PGA2	Oxylipin	-0.1023	0.4090	-0.2500	8.0258E-01	9.7762E-01
LPI (14:0)	Lysophospholipid	-0.1469	0.6142	-0.2393	8.1090E-01	9.8372E-01
2-aminoadipic acid	Amine	-0.1403	0.6134	-0.2288	8.1905E-01	9.8908E-01
12-HHTrE/AA	Oxylipin	-0.0669	0.2973	-0.2250	8.2200E-01	9.8908E-01
TXB1	Oxylipin	-0.0751	0.3678	-0.2041	8.3831E-01	9.9192E-01
20-HETE/AA	Oxylipin	-0.1816	0.9480	-0.1916	8.4809E-01	9.9192E-01

LPA (18:0)	Lysophospholipid	-0.1742	0.9125	-0.1909	8.4861E-01	9.9192E-01
Clupanodonic acid	Fatty acid	0.0637	0.3394	0.1876	8.5123E-01	9.9192E-01
PGF2alpha	Oxylipin	0.0554	0.2968	0.1868	8.5184E-01	9.9192E-01
9-HODE	Oxylipin	0.0835	0.4479	0.1865	8.5204E-01	9.9192E-01
PGF2alpha/AA	Oxylipin	0.0545	0.2986	0.1825	8.5516E-01	9.9192E-01
PGE1/DGLA	Oxylipin	-0.0506	0.2796	-0.1808	8.5654E-01	9.9192E-01
Putrescine	Amine	0.0480	0.2784	0.1726	8.6300E-01	9.9192E-01
14,15-DiHETE	Oxylipin	-0.0844	0.4938	-0.1710	8.6423E-01	9.9192E-01
12-HHTrE	Oxylipin	-0.0451	0.2728	-0.1653	8.6871E-01	9.9192E-01
9-KODE	Oxylipin	0.0794	0.4809	0.1650	8.6893E-01	9.9192E-01
1-Met-His	Amine	0.2620	1.7568	0.1491	8.8145E-01	9.9192E-01
8-HDoHE	Oxylipin	0.0627	0.4342	0.1444	8.8515E-01	9.9192E-01
Asp	Amine	-0.1148	0.8001	-0.1434	8.8595E-01	9.9192E-01
5-HETrE/DGLA	Oxylipin	0.0498	0.3775	0.1320	8.9499E-01	9.9192E-01
FA (16:0)	Fatty acid	0.0802	0.6116	0.1311	8.9569E-01	9.9192E-01
16-HDoHE	Oxylipin	0.0558	0.4545	0.1228	9.0229E-01	9.9192E-01
Homocitrulline	Amine	0.0978	0.8020	0.1220	9.0291E-01	9.9192E-01
9-HOTrE/ALA	Oxylipin	-0.0707	0.5987	-0.1181	9.0596E-01	9.9192E-01
TXB2	Oxylipin	0.0333	0.2878	0.1158	9.0778E-01	9.9192E-01
AA	Fatty acid	0.0880	0.7701	0.1143	9.0902E-01	9.9192E-01
5-HEPE	Oxylipin	0.0576	0.5168	0.1114	9.1131E-01	9.9192E-01
7-HDoHE/DHA	Oxylipin	-0.0511	0.4791	-0.1067	9.1503E-01	9.9192E-01
2,3-dinor-8-iso-PGF2alpha/AA	Oxylipin	0.0356	0.3371	0.1056	9.1587E-01	9.9192E-01
Ornithine/Arg	Amine	-0.0618	0.5961	-0.1037	9.1743E-01	9.9192E-01
8-iso-PGF3alpha/DGLA	Oxylipin	0.0143	0.1517	0.0943	9.2485E-01	9.9192E-01
LPA (18:1)	Lysophospholipid	0.0722	0.7960	0.0906	9.2777E-01	9.9192E-01
19,20-DiHDPA/19,20-EpDPE	Oxylipin	-0.0367	0.4149	-0.0885	9.2946E-01	9.9192E-01
8-iso-PGF3alpha	Oxylipin	0.0144	0.1632	0.0880	9.2985E-01	9.9192E-01
3-Met-His	Amine	0.0762	0.9104	0.0836	9.3334E-01	9.9192E-01
GABA	Amine	0.0620	0.7765	0.0799	9.3634E-01	9.9192E-01
TXB2/AA	Oxylipin	0.0240	0.3073	0.0780	9.3781E-01	9.9192E-01
5-KETE	Oxylipin	-0.0487	0.6289	-0.0774	9.3830E-01	9.9192E-01
2,3-dinor-8-iso-PGF2alpha	Oxylipin	-0.0227	0.3676	-0.0617	9.5077E-01	9.9709E-01
ETE	Fatty acid	0.0383	0.6873	0.0558	9.5552E-01	9.9709E-01
9-KODE/9-HODE	Oxylipin	-0.0405	0.7526	-0.0538	9.5712E-01	9.9709E-01
15-HETE	Oxylipin	0.0214	0.4300	0.0498	9.6026E-01	9.9709E-01
20-HETE	Oxylipin	-0.0388	0.8460	-0.0458	9.6343E-01	9.9709E-01
LA	Fatty acid	0.0329	0.7773	0.0423	9.6627E-01	9.9709E-01
PGE2	Oxylipin	0.0120	0.3085	0.0390	9.6887E-01	9.9709E-01
Sum HETEs	Oxylipin	0.0167	0.5229	0.0319	9.7454E-01	9.9709E-01
LPA (16:0)	Lysophospholipid	-0.0211	0.6626	-0.0318	9.7461E-01	9.9709E-01
AABA	Amine	0.0124	0.4854	0.0256	9.7960E-01	9.9709E-01
AEA	Endocannabinoid	0.0150	0.6875	0.0217	9.8265E-01	9.9709E-01
15-HETE/AA	Oxylipin	-0.0102	0.5561	-0.0183	9.8541E-01	9.9709E-01
PGE2/AA	Oxylipin	-0.0025	0.3363	-0.0074	9.9406E-01	9.9709E-01
12-KETE	Oxylipin	0.0018	0.2769	0.0064	9.9486E-01	9.9709E-01
Gly-Gly	Amine	-0.0015	0.4093	-0.0038	9.9701E-01	9.9709E-01
TXB1/DGLA	Oxylipin	0.0012	0.3241	0.0036	9.9709E-01	9.9709E-01

Table S12: Logistic regression results of the "C_S" model comparing control with sepsis in the single time point dataset

Metabolite	Category	Estimate	Standard Error	z-value	p-value	Adjusted p-value
Cortisol	Steroid Hormone	2.4649	0.6828	3.6100	3.0624E-04	2.9972E-02
Trp	Amine	-7.3939	2.1099	-3.5043	4.5783E-04	2.9972E-02
Phe/Tyr	Amine	4.4600	1.2916	3.4532	5.5399E-04	2.9972E-02
LPS (18:0)	Lysophospholipid	1.8944	0.5565	3.4038	6.6458E-04	2.9972E-02
Arg	Amine	-2.5011	0.7514	-3.3287	8.7257E-04	2.9972E-02
LPI (18:0)	Lysophospholipid	5.2127	1.5702	3.3198	9.0072E-04	2.9972E-02
Tyr	Amine	-2.5775	0.7784	-3.3114	9.2819E-04	2.9972E-02
BCAA/Tyr	Amine	3.2299	0.9819	3.2894	1.0039E-03	2.9972E-02
Met	Amine	-5.2608	1.6041	-3.2797	1.0393E-03	2.9972E-02
Gln	Amine	-2.7578	0.8513	-3.2397	1.1966E-03	2.9972E-02
Thr	Amine	-2.8680	0.8896	-3.2239	1.2646E-03	2.9972E-02
LPI (16:0)	Lysophospholipid	4.1696	1.2968	3.2154	1.3027E-03	2.9972E-02
AAA	Amine	-3.7987	1.1825	-3.2124	1.3163E-03	2.9972E-02
SIP (18:2)	Lysophospholipid	-3.1998	1.0396	-3.0780	2.0837E-03	4.3238E-02
LPE (16:0)	Lysophospholipid	3.2454	1.0595	3.0630	2.1911E-03	4.3238E-02
BCAA/AAA	Amine	4.0600	1.3409	3.0279	2.4625E-03	4.5566E-02
OH-Lys	Amine	-3.1611	1.0607	-2.9802	2.8803E-03	5.0150E-02
Ser	Amine	-3.1943	1.0991	-2.9064	3.6556E-03	6.0115E-02
SIP (18:1)	Lysophospholipid	-2.5280	0.8840	-2.8597	4.2398E-03	6.4383E-02
4-OH-Pro/Pro	Amine	-2.9147	1.0221	-2.8516	4.3502E-03	6.4383E-02

Chapter III

ADMA	Amine	-2.8487	1.0130	-2.8122	4.9200E-03	6.9348E-02
Ile	Amine	-3.4671	1.2669	-2.7366	6.2071E-03	7.9857E-02
LPE (20:4)	Lysophospholipid	-2.5446	0.9331	-2.7271	6.3898E-03	7.9857E-02
LPE (22:4)	Lysophospholipid	-1.7937	0.6592	-2.7208	6.5115E-03	7.9857E-02
Lys	Amine	-3.2104	1.1850	-2.7092	6.7446E-03	7.9857E-02
g-Glu-Gln	Amine	-1.1683	0.4374	-2.6708	7.5668E-03	8.6145E-02
3-Methoxy-tyrosine	Amine	-1.7495	0.6725	-2.6016	9.2780E-03	1.0012E-01
4-OH-Pro	Amine	-2.4912	0.9601	-2.5946	9.4707E-03	1.0012E-01
Asn	Amine	-2.7264	1.0632	-2.5642	1.0341E-02	1.0048E-01
LPS (22:4)	Lysophospholipid	1.8696	0.7333	2.5494	1.0790E-02	1.0048E-01
LPE (22:6)	Lysophospholipid	-2.6916	1.0565	-2.5477	1.0845E-02	1.0048E-01
His	Amine	-2.7008	1.0637	-2.5391	1.1115E-02	1.0048E-01
Citrulline	Amine	-1.8822	0.7422	-2.5360	1.1212E-02	1.0048E-01
Leu	Amine	-3.5243	1.3953	-2.5258	1.1542E-02	1.0048E-01
Ornithine	Amine	-1.8321	0.7316	-2.5043	1.2268E-02	1.0340E-01
Gln/Glu	Amine	-1.1992	0.4805	-2.4956	1.2576E-02	1.0340E-01
5-KETE/5-HETE	Oxylipin	1.5209	0.6144	2.4753	1.3313E-02	1.0650E-01
LPE (20:3)	Lysophospholipid	-2.0612	0.8524	-2.4179	1.5609E-02	1.1165E-01
cLPA (20:4)	Lysophospholipid	-1.1191	0.4632	-2.4162	1.5683E-02	1.1165E-01
Sum OG	Endocannabinoid	-1.2027	0.4989	-2.4109	1.5911E-02	1.1165E-01
DHEA	Endocannabinoid	1.7554	0.7283	2.4102	1.5944E-02	1.1165E-01
Arg/Lys	Amine	-1.6309	0.6780	-2.4056	1.6146E-02	1.1165E-01
BCAA	Amine	-3.0923	1.2863	-2.4039	1.6219E-02	1.1165E-01
DEA	Endocannabinoid	1.0757	0.4550	2.3639	1.8082E-02	1.2165E-01
Saccharopine	Amine	-1.1092	0.4750	-2.3353	1.9527E-02	1.2844E-01
18-HEPE	Oxylipin	0.9643	0.4182	2.3058	2.1124E-02	1.3490E-01
LA	Fatty acid	2.3874	1.0378	2.3005	2.1421E-02	1.3490E-01
GABA	Amine	1.4895	0.6625	2.2484	2.4551E-02	1.5140E-01
LPI (14:0)	Lysophospholipid	1.3006	0.5842	2.2264	2.5985E-02	1.5463E-01
Gly-Pro	Amine	-1.1319	0.5088	-2.2244	2.6121E-02	1.5463E-01
LPE (18:0)	Lysophospholipid	1.7948	0.8168	2.1974	2.7990E-02	1.6038E-01
LPI (16:1)	Lysophospholipid	1.3016	0.5968	2.1811	2.9180E-02	1.6038E-01
5-HEPE/EPA	Oxylipin	-1.1865	0.5442	-2.1804	2.9231E-02	1.6038E-01
LPS (18:2)	Lysophospholipid	1.2535	0.5750	2.1800	2.9258E-02	1.6038E-01
Glu/GABA	Amine	-1.5176	0.7131	-2.1281	3.3329E-02	1.7937E-01
LPS (16:0)	Lysophospholipid	3.7997	1.8050	3.5277E-02	3.8647E-01	
EPA	Fatty acid	0.8323	0.3994	2.0837	3.7186E-02	1.9070E-01
Putrescine	Amine	1.0008	0.4807	2.0817	3.7367E-02	1.9070E-01
Gly	Amine	-2.5742	1.2907	-1.9945	4.6101E-02	2.2851E-01
Val	Amine	-2.3473	1.1781	-1.9925	4.6319E-02	2.2851E-01
5-HETE/AA	Oxylipin	-1.2540	0.6384	-1.9642	4.9502E-02	2.4020E-01
5-HT/Trp	Amine	0.4444	0.2277	1.9520	5.0935E-02	2.4317E-01
LPI (18:1)	Lysophospholipid	1.4695	0.7761	1.8934	5.8309E-02	2.7396E-01
3-AIBA	Amine	0.8439	0.4537	1.8602	6.2860E-02	2.9027E-01
LPE (18:2)	Lysophospholipid	-1.3285	0.7166	-1.8540	6.3741E-02	2.9027E-01
12,13-EpOME/LA	Oxylipin	-0.9056	0.4908	-1.8453	6.4996E-02	2.9150E-01
LPA (20:4)	Lysophospholipid	-1.2031	0.6599	-1.8232	6.8276E-02	2.9954E-01
11beta-PGF2alpha	Oxylipin	0.5927	0.3279	1.8075	7.0682E-02	2.9954E-01
S-Methyl-Cys	Amine	-1.8942	1.0487	-1.8062	7.0880E-02	2.9954E-01
LPE (20:5)	Lysophospholipid	-1.9784	1.0963	-1.8047	7.1127E-02	2.9954E-01
Sphinganine 18.0	Lysophospholipid	0.8493	0.4718	1.8001	7.1850E-02	2.9954E-01
5-iPF2alpha-VI	Oxylipin	1.0602	0.6038	1.7560	7.9087E-02	3.1986E-01
Sarcosine	Amine	-0.8173	0.4662	-1.7529	7.9619E-02	3.1986E-01
S1P (16:1)	Lysophospholipid	-1.2168	0.6971	-1.7456	8.0883E-02	3.1986E-01
Sum DiHETrEs	Oxylipin	-0.9872	0.5670	-1.7411	8.1664E-02	3.1986E-01
9-HOTrE/ALA	Oxylipin	-0.8177	0.4714	-1.7345	8.2834E-02	3.1986E-01
cLPA (18:2)	Lysophospholipid	-0.6566	0.3790	-1.7324	8.3207E-02	3.1986E-01
Arg/ADMA	Amine	-0.9634	0.5673	-1.6982	8.9471E-02	3.3953E-01
ALA	Fatty acid	0.8991	0.5350	1.6807	9.2819E-02	3.4778E-01
5-KETE	Oxylipin	0.9899	0.5953	1.6629	9.6331E-02	3.5566E-01
14,15-DiHETrE	Oxylipin	-0.9252	0.5580	-1.6580	9.7325E-02	3.5566E-01
Homoserine	Amine	-1.4345	0.8765	-1.6366	1.0172E-01	3.6719E-01
HCA	Bile Acid	-0.2461	0.1509	-1.6303	1.0303E-01	3.6743E-01
5-HETrE/DGLA	Oxylipin	-0.6279	0.3870	-1.6223	1.0474E-01	3.6875E-01
TUDCA	Bile Acid	0.3436	0.2125	1.6169	1.0589E-01	3.6875E-01
8,9-DiHETrE	Oxylipin	-0.7118	0.4498	-1.5825	1.1354E-01	3.9080E-01
LPA (22:4)	Lysophospholipid	-0.8366	0.5334	-1.5686	1.1674E-01	3.9111E-01
LPA (20:3)	Lysophospholipid	-0.8946	0.5705	-1.5680	1.1688E-01	3.9111E-01
SDMA	Amine	-1.4023	0.8977	-1.5620	1.1828E-01	3.9111E-01
S1P (18:0)	Lysophospholipid	-0.9175	0.5889	-1.5578	1.1927E-01	3.9111E-01
11,12-DiHETrE	Oxylipin	-0.7910	0.5103	-1.5502	1.2110E-01	3.9111E-01
Sum iPs	Oxylipin	0.2574	0.1669	1.5421	1.2305E-01	3.9111E-01
AEA	Endocannabinoid	1.0419	0.6772	1.5384	1.2395E-01	3.9111E-01
8-iso-PGF3alpha	Oxylipin	0.2284	0.1490	1.5324	1.2542E-01	3.9111E-01

Diagnosis of Late-Onset Sepsis

20-HDoHE	Oxylipin	0.6856	0.4475	1.5320	1.2552E-01	3.9111E-01
Ornithine/Arg	Amine	0.6799	0.4538	1.4982	1.3407E-01	4.1339E-01
Sum HEPeS	Oxylipin	0.3675	0.2490	1.4758	1.4001E-01	4.2723E-01
12-HEPE	Oxylipin	0.3734	0.2578	1.4482	1.4757E-01	4.4572E-01
PAF 16(0)	PAF	-0.5779	0.4064	-1.4219	1.5506E-01	4.5989E-01
11beta-PGF2alpha/AA	Oxylipin	0.3949	0.2794	1.4134	1.5754E-01	4.5989E-01
cLPA (18:1)	Lysophospholipid	-0.5450	0.3861	-1.4115	1.5809E-01	4.5989E-01
LCA	Bile Acid	-1.3267	0.9407	-1.4102	1.5847E-01	4.5989E-01
Trimethyl-Lys	Amine	-1.3536	0.9728	-1.3915	1.6408E-01	4.7154E-01
5-HETE	Oxylipin	-0.7240	0.5282	-1.3707	1.7047E-01	4.7771E-01
Sphingosine 18.1	Lysophospholipid	0.5899	0.4311	1.3683	1.7122E-01	4.7771E-01
PGe1	Oxylipin	0.3944	0.2884	1.3677	1.7140E-01	4.7771E-01
15-HEPE/EPA	Oxylipin	-0.6906	0.5064	-1.3636	1.7269E-01	4.7771E-01
LPS (22:6)	Lysophospholipid	0.6858	0.5063	1.3546	1.7556E-01	4.7983E-01
3-Methoxy-tyramine	Amine	1.4621	1.0822	1.3510	1.7669E-01	4.7983E-01
cLPA (16:1)	Lysophospholipid	-1.0358	0.7771	-1.3330	1.8252E-01	4.9116E-01
EA	Amine	0.8700	0.6716	1.2953	1.9520E-01	5.1842E-01
20-HETE/AA	Oxylipin	-0.9081	0.7025	-1.2926	1.9616E-01	5.1842E-01
9-HEPE	Oxylipin	0.4482	0.3506	1.2785	2.0107E-01	5.2668E-01
TXB3/EPA	Oxylipin	-0.2869	0.2266	-1.2659	2.0556E-01	5.3373E-01
LPG (18:1)	Lysophospholipid	-1.2953	1.0479	-1.2361	2.1642E-01	5.5618E-01
Met-SO	Amine	-1.0575	0.8584	-1.2320	2.1796E-01	5.5618E-01
delta-17,6-keto-PGF1alpha/EPA	Oxylipin	-0.1842	0.1502	-1.2265	2.2001E-01	5.5606E-01
5-iPF2alpha-VI/AA	Oxylipin	0.6219	0.5161	1.2051	2.2817E-01	5.6970E-01
Met-SO2	Amine	-0.6126	0.5094	-1.2026	2.2915E-01	5.6970E-01
LPG (16:0)	Lysophospholipid	1.0264	0.8569	1.1979	2.3096E-01	5.6970E-01
Coriolic acid	Oxylipin	0.4925	0.4155	1.1856	2.3579E-01	5.7290E-01
5,6-DiHETE	Oxylipin	-0.3852	0.3257	-1.1827	2.3691E-01	5.7290E-01
8-iso-PGF3alpha/DGLA	Oxylipin	0.1627	0.1379	1.1798	2.3806E-01	5.7290E-01
Kyn/Trp	Amine	0.5366	0.4598	1.1670	2.4321E-01	5.7820E-01
Kyn	Amine	-0.5068	0.4352	-1.1646	2.4417E-01	5.7820E-01
8,12-iso-iPF2alpha-VI/AA	Oxylipin	-0.7090	0.6212	-1.1413	2.5374E-01	5.9249E-01
Sum HODEs	Oxylipin	0.4911	0.4307	1.1402	2.5421E-01	5.9249E-01
2,3-dinor-8-iso-PGF2alpha	Oxylipin	0.3512	0.3097	1.1341	2.5674E-01	5.9371E-01
1-Met-His	Amine	-2.4834	2.2098	-1.1238	2.6109E-01	5.9909E-01
19,20-DiHDDPA/19,20-EpDPE	Oxylipin	-0.4834	0.4335	-1.1151	2.6481E-01	6.0013E-01
Anserine	Amine	-0.5443	0.4896	-1.1117	2.6626E-01	6.0013E-01
LPG (18:3)	Lysophospholipid	0.5945	0.5364	1.1085	2.6766E-01	6.0013E-01
15-HEPE	Oxylipin	0.4216	0.3819	1.1039	2.6965E-01	6.0013E-01
LPA (20:5)	Lysophospholipid	0.4660	0.4267	1.0922	2.7476E-01	6.0693E-01
15-HETE	Oxylipin	0.3828	0.3541	1.0810	2.7969E-01	6.1051E-01
12-HHTrE/AA	Oxylipin	-0.2687	0.2497	-1.0759	2.8197E-01	6.1051E-01
5-HETE	Oxylipin	-0.4370	0.4067	-1.0746	2.8257E-01	6.1051E-01
9-HEPE/EPA	Oxylipin	-0.5531	0.5204	-1.0629	2.8784E-01	6.1556E-01
5-HT	Amine	0.2211	0.2101	1.0523	2.9265E-01	6.1556E-01
LPI (18:2)	Lysophospholipid	0.6957	0.6612	1.0522	2.9270E-01	6.1556E-01
LPE (14:0)	Lysophospholipid	0.6319	0.6012	1.0511	2.9322E-01	6.1556E-01
w3FA/w6FA	Fatty acid	0.6457	0.6176	1.0455	2.9577E-01	6.1654E-01
Carnosine	Amine	-0.4095	0.3962	-1.0337	3.0130E-01	6.2343E-01
Clupanodonic acid	Fatty acid	0.3334	0.3246	1.0272	3.0431E-01	6.2343E-01
7-HDoHE/DHA	Oxylipin	-0.4999	0.4877	-1.0249	3.0540E-01	6.2343E-01
9-HODE	Oxylipin	0.4307	0.4297	1.0024	3.1613E-01	6.3779E-01
14,15-DiHETE	Oxylipin	0.4412	0.4407	1.0012	3.1674E-01	6.3779E-01
11-HETE/AA	Oxylipin	-0.4764	0.4902	-0.9718	3.3117E-01	6.6235E-01
20-HDoHE/DHA	Oxylipin	0.4255	0.4498	0.9459	3.4420E-01	6.8242E-01
LPE (18:1)	Lysophospholipid	-0.5777	0.6128	-0.9427	3.4582E-01	6.8242E-01
2,3-dinor-8-iso-PGF2alpha/AA	Oxylipin	0.2695	0.2875	0.9375	3.4853E-01	6.8320E-01
LPA (18:2)	Lysophospholipid	-0.5885	0.6374	-0.9232	3.5590E-01	6.9307E-01
OA	Fatty acid	-1.3000	1.4428	-0.9010	3.6757E-01	7.0823E-01
HomoCys	Amine	-0.4101	0.4560	-0.8993	3.6847E-01	7.0823E-01
12-HHTrE	Oxylipin	-0.2189	0.2474	-0.8848	3.7627E-01	7.1574E-01
TLCA-3S	Bile Acid	-0.2005	0.2278	-0.8800	3.7884E-01	7.1574E-01
g-Glu-Ala	Amine	-0.3877	0.4434	-0.8743	3.8196E-01	7.1574E-01
AABA	Amine	0.4592	0.5253	0.8741	3.8205E-01	7.1574E-01
LPG (14:0)	Lysophospholipid	0.4767	0.5506	0.8658	3.8658E-01	7.1967E-01
OH-Lys/Lys	Amine	-0.6686	0.7805	-0.8566	3.9167E-01	7.2231E-01
LPA (18:1)	Lysophospholipid	-0.4802	0.5630	-0.8529	3.9369E-01	7.2231E-01
19,20-DiHDDPA	Oxylipin	-0.3958	0.4656	-0.8500	3.9532E-01	7.2231E-01
11,12-DiHETrE/11,12-EpETrE	Oxylipin	-0.3080	0.3675	-0.8381	4.0198E-01	7.2558E-01
Sum HDoHEs	Oxylipin	0.2658	0.3172	0.8380	4.0201E-01	7.2558E-01
20-HETE	Oxylipin	-0.5504	0.6640	-0.8290	4.0708E-01	7.3028E-01
14-HDoHE	Oxylipin	0.2200	0.2676	0.8220	4.1107E-01	7.3300E-01
Sum AG	Endocannabinoid	-0.2760	0.3387	-0.8149	4.1515E-01	7.3447E-01
Sum LG	Endocannabinoid	-0.3491	0.4321	-0.8078	4.1922E-01	7.3447E-01

Chapter III

LPS (18:1)	Lysosphospholipid	0.3786	0.4688	0.8076	4.1934E-01	7.3447E-01
11,12-EpETrE/AA	Oxylipin	-0.3794	0.4814	-0.7881	4.3063E-01	7.4634E-01
17,18-DiHETE	Oxylipin	-0.2163	0.2754	-0.7855	4.3216E-01	7.4634E-01
Sum PGs	Oxylipin	-0.1871	0.2389	-0.7829	4.3369E-01	7.4634E-01
Homocitrulline	Amine	-0.4542	0.5836	-0.7783	4.3641E-01	7.4669E-01
2-aminoadipic acid	Amine	-0.3748	0.4962	-0.7553	4.5004E-01	7.6484E-01
FA (16:0)	Fatty acid	-0.5013	0.6668	-0.7518	4.5218E-01	7.6484E-01
LPA (22:6)	Lysosphospholipid	-0.4086	0.5469	-0.7471	4.5497E-01	7.6518E-01
PGF1alpha	Oxylipin	-0.1565	0.2130	-0.7347	4.6253E-01	7.6978E-01
Sum HETrEs	Oxylipin	0.2697	0.3674	0.7341	4.6291E-01	7.6978E-01
PGA2/AA	Oxylipin	-0.2407	0.3321	-0.7248	4.6856E-01	7.7483E-01
12,13-EpOME	Oxylipin	-0.3294	0.4619	-0.7132	4.7570E-01	7.7913E-01
8-HETrE	Oxylipin	0.2416	0.3416	0.7072	4.7941E-01	7.7913E-01
CA	Bile Acid	-0.1295	0.1832	-0.7066	4.7980E-01	7.7913E-01
9-KODE	Oxylipin	0.2859	0.4064	0.7036	4.8169E-01	7.7913E-01
9-HpODE/LA	Oxylipin	-0.2534	0.3642	-0.6959	4.8649E-01	7.8098E-01
DGLA	Fatty acid	0.2912	0.4200	0.6933	4.8811E-01	7.8098E-01
LPG (18:0)	Lysosphospholipid	0.5119	0.7553	0.6778	4.9792E-01	7.9239E-01
11-HDoHE	Oxylipin	0.1995	0.2982	0.6691	5.0346E-01	7.9692E-01
THDCA	Bile Acid	0.1485	0.2257	0.6581	5.1047E-01	7.9916E-01
Sum SBA	Bile Acid	0.4072	0.6212	0.6556	5.1211E-01	7.9916E-01
DPA	Fatty acid	-0.2357	0.3637	-0.6481	5.1689E-01	7.9916E-01
PGA2	Oxylipin	-0.1748	0.2709	-0.6453	5.1875E-01	7.9916E-01
17-HDoHE	Oxylipin	0.2281	0.3550	0.6426	5.2048E-01	7.9916E-01
LPG (22:6)	Lysosphospholipid	0.3303	0.5147	0.6417	5.2107E-01	7.9916E-01
Sum BA	Bile Acid	-0.0821	0.1294	-0.6343	5.2591E-01	8.0241E-01
Phe	Amine	-0.5824	0.9357	-0.6224	5.3368E-01	8.0368E-01
LPE (16:1)	Lysosphospholipid	-0.3753	0.6046	-0.6208	5.3473E-01	8.0368E-01
8,12-iso-iPF2alpha-VI	Oxylipin	-0.3247	0.5241	-0.6195	5.3556E-01	8.0368E-01
Sum PBA	Bile Acid	-0.0896	0.1478	-0.6061	5.4447E-01	8.0368E-01
DHA	Fatty acid	0.2509	0.4145	0.6053	5.4496E-01	8.0368E-01
LPG (22:4)	Lysosphospholipid	0.4239	0.7089	0.5979	5.4991E-01	8.0368E-01
O-PO3-EA	Amine	0.2205	0.3696	0.5967	5.5069E-01	8.0368E-01
Cystathionine/HomoCys	Amine	0.1850	0.3104	0.5962	5.5106E-01	8.0368E-01
TCA	Bile Acid	0.0949	0.1593	0.5960	5.5117E-01	8.0368E-01
15-HETrE/DGLA	Oxylipin	0.1993	0.3664	0.5441	5.8635E-01	8.5046E-01
10-HDoHE	Oxylipin	0.1954	0.3627	0.5386	5.9019E-01	8.5046E-01
ETE	Fatty acid	0.3209	0.5995	0.5353	5.9247E-01	8.5046E-01
Sum DiHETEs	Oxylipin	-0.1687	0.3172	-0.5320	5.9475E-01	8.5046E-01
cLPA (14:0)	Lysosphospholipid	-0.2897	0.5760	-0.5029	6.1507E-01	8.6407E-01
9-KODE/9-HODE	Oxylipin	-0.4044	0.8085	-0.5001	6.1698E-01	8.6407E-01
cLPA (18:0)	Lysosphospholipid	0.2344	0.4718	0.4968	6.1933E-01	8.6407E-01
11-HETE	Oxylipin	-0.1942	0.3919	-0.4956	6.2017E-01	8.6407E-01
LPA (16:0)	Lysosphospholipid	-0.2367	0.4786	-0.4945	6.2097E-01	8.6407E-01
LPA (22:5)	Lysosphospholipid	0.2433	0.4938	0.4927	6.2226E-01	8.6407E-01
AA	Fatty acid	0.3212	0.6565	0.4892	6.2470E-01	8.6407E-01
16-HDoHE/DHA	Oxylipin	-0.2758	0.5694	-0.4843	6.2818E-01	8.6484E-01
14-HDoHE/DHA	Oxylipin	0.1376	0.2964	0.4643	6.4245E-01	8.7840E-01
Sum HETEs	Oxylipin	-0.2305	0.5008	-0.4602	6.4538E-01	8.7840E-01
LPA (14:0)	Lysosphospholipid	0.1865	0.4071	0.4580	6.4693E-01	8.7840E-01
LPG (16:1)	Lysosphospholipid	0.2378	0.5261	0.4519	6.5131E-01	8.8031E-01
Cys	Amine	-0.2163	0.4919	-0.4396	6.6020E-01	8.8827E-01
Mead.Acid	Fatty acid	-0.1475	0.3514	-0.4198	6.7464E-01	8.9946E-01
LPG (20:4)	Lysosphospholipid	-0.3204	0.7756	-0.4131	6.7956E-01	8.9946E-01
12,13-DiHOME	Oxylipin	-0.1558	0.3801	-0.4098	6.8196E-01	8.9946E-01
13-HDoHE	Oxylipin	0.1581	0.3883	0.4072	6.8384E-01	8.9946E-01
8-HDoHE	Oxylipin	0.1560	0.3897	0.4002	6.8897E-01	8.9946E-01
PGE2/AA	Oxylipin	-0.0974	0.2436	-0.3999	6.8925E-01	8.9946E-01
19,20-EpDPE	Oxylipin	0.1806	0.4524	0.3991	6.8979E-01	8.9946E-01
5-HEPE	Oxylipin	0.1686	0.4509	0.3738	7.0855E-01	9.1439E-01
11,12-EpETrE	Oxylipin	-0.1507	0.4053	-0.3719	7.0999E-01	9.1439E-01
13,14-dihydro-15-keto-PGF2alpha	Oxylipin	0.1059	0.2853	0.3712	7.1051E-01	9.1439E-01
PGE2	Oxylipin	-0.0818	0.2302	-0.3554	7.2231E-01	9.2556E-01
9-HpODE	Oxylipin	0.1234	0.3541	0.3485	7.2744E-01	9.2812E-01
LPE (18:3)	Lysosphospholipid	0.1165	0.3446	0.3380	7.3536E-01	9.3420E-01
TXBI/DGLA	Oxylipin	-0.0824	0.2554	-0.3225	7.4706E-01	9.4025E-01
15-HETE	Oxylipin	0.1237	0.3837	0.3223	7.4719E-01	9.4025E-01
TXB1	Oxylipin	0.0959	0.3006	0.3191	7.4966E-01	9.4025E-01
beta-Ala	Amine	0.2757	0.9046	0.3048	7.6055E-01	9.4989E-01
Citrulline/Ornithine	Amine	-0.1527	0.5333	-0.2862	7.7471E-01	9.6185E-01
7-HDoHE	Oxylipin	-0.1058	0.3813	-0.2774	7.8146E-01	9.6185E-01
Tau	Amine	0.1575	0.5820	0.2706	7.8672E-01	9.6185E-01
GLA	Fatty acid	0.1951	0.7296	0.2674	7.8915E-01	9.6185E-01
19,20-EpDPE/DHA	Oxylipin	-0.1214	0.4658	-0.2606	7.9441E-01	9.6185E-01

11-HDoHE/DHA	Oxylipin	0.0912	0.3519	0.2592	7.9549E-01	9.6185E-01
16-HDoHE	Oxylipin	0.1102	0.4277	0.2575	7.9676E-01	9.6185E-01
Cys/Cystathionine	Amine	-0.0802	0.3195	-0.2512	8.0169E-01	9.6185E-01
Pro	Amine	0.3065	1.2202	0.2512	8.0169E-01	9.6185E-01
O-Acetyl-Ser	Amine	-0.1332	0.5418	-0.2459	8.0576E-01	9.6185E-01
LPI (22:4)	Lysophospholipid	-0.1541	0.6385	-0.2413	8.0931E-01	9.6185E-01
TXB2/AA	Oxylipin	-0.0594	0.2524	-0.2352	8.1405E-01	9.6185E-01
LPS (20:4)	Lysophospholipid	-0.1165	0.4961	-0.2349	8.1432E-01	9.6185E-01
9-HOTrE	Oxylipin	-0.0823	0.3530	-0.2332	8.1563E-01	9.6185E-01
8-HDoHE/DHA	Oxylipin	-0.1235	0.5423	-0.2278	8.1982E-01	9.6203E-01
12-KETE/12-HETE	Oxylipin	0.0560	0.2519	0.2224	8.2397E-01	9.6203E-01
GCA	Bile Acid	-0.0305	0.1385	-0.2202	8.2568E-01	9.6203E-01
Ada	Fatty acid	-0.0973	0.4499	-0.2163	8.2878E-01	9.6203E-01
13-HDoHE/DHA	Oxylipin	-0.1029	0.5023	-0.2049	8.3764E-01	9.6321E-01
12,13-DiHOME/12,13-EpOME	Oxylipin	0.0812	0.4061	0.2000	8.4147E-01	9.6321E-01
LPA (16:1)	Lysophospholipid	0.0797	0.3992	0.1998	8.4166E-01	9.6321E-01
LPG (18:2)	Lysophospholipid	-0.1180	0.6128	-0.1925	8.4734E-01	9.6321E-01
PGF2alpha	Oxylipin	0.0457	0.2414	0.1893	8.4989E-01	9.6321E-01
Glu	Amine	0.1370	0.7395	0.1852	8.5308E-01	9.6321E-01
12-KETE	Oxylipin	-0.0418	0.2303	-0.1814	8.5605E-01	9.6321E-01
13,14-dihydro-15-keto-PGF2alpha/AA	Oxylipin	0.0553	0.3149	0.1756	8.6058E-01	9.6321E-01
Asp	Amine	0.0965	0.5598	0.1724	8.6316E-01	9.6321E-01
12-HETE/AA	Oxylipin	-0.0480	0.2942	-0.1632	8.7039E-01	9.6321E-01
PGF1alpha/DGLA	Oxylipin	-0.0288	0.1765	-0.1629	8.7059E-01	9.6321E-01
3-Met-His	Amine	-0.0926	0.5785	-0.1600	8.7287E-01	9.6321E-01
8-HETrE/DGLA	Oxylipin	0.0548	0.3552	0.1544	8.7728E-01	9.6321E-01
9-HODE/9-HpODE	Oxylipin	-0.0784	0.5111	-0.1534	8.7809E-01	9.6321E-01
PGF2alpha/AA	Oxylipin	0.0370	0.2441	0.1518	8.7936E-01	9.6321E-01
17-HDoHE/DHA	Oxylipin	0.0681	0.4581	0.1486	8.8186E-01	9.6321E-01
LPG (20:3)	Lysophospholipid	0.1362	0.9467	0.1439	8.8560E-01	9.6374E-01
18-HEPE/EPA	Oxylipin	0.0408	0.3126	0.1305	8.9613E-01	9.7163E-01
PAF 18(2)	PAF	-0.0271	0.2283	-0.1188	9.0540E-01	9.7810E-01
LPA (18:0)	Lysophospholipid	-0.0717	0.6487	-0.1105	9.1198E-01	9.8163E-01
delta-17,6-keto-PGF1alpha	Oxylipin	-0.0202	0.1913	-0.1054	9.1607E-01	9.8245E-01
PGE1/DGLA	Oxylipin	-0.0259	0.2595	-0.0999	9.2041E-01	9.8300E-01
Sum KETEs	Oxylipin	0.0252	0.2611	0.0964	9.2323E-01	9.8300E-01
LPI (22:6)	Lysophospholipid	-0.0564	0.7832	-0.0720	9.4257E-01	9.9011E-01
12-HEPE/EPA	Oxylipin	-0.0206	0.3076	-0.0669	9.4668E-01	9.9011E-01
TXB3	Oxylipin	-0.0108	0.2056	-0.0524	9.5824E-01	9.9011E-01
5-aminolevulinic acid	Amine	-0.0327	0.6252	-0.0522	9.5833E-01	9.9011E-01
Sum TxS	Oxylipin	-0.0119	0.2318	-0.0515	9.5893E-01	9.9011E-01
12-HETE	Oxylipin	0.0129	0.2586	0.0500	9.6009E-01	9.9011E-01
15-HETE/AA	Oxylipin	0.0228	0.4989	0.0457	9.6354E-01	9.9011E-01
FA (18:0)	Fatty acid	-0.0351	0.7697	-0.0455	9.6368E-01	9.9011E-01
TXB2	Oxylipin	-0.0110	0.2450	-0.0448	9.6424E-01	9.9011E-01
GCDCa	Bile Acid	0.0056	0.1275	0.0437	9.6514E-01	9.9011E-01
Cystathionine	Amine	-0.0141	0.3642	-0.0388	9.6904E-01	9.9011E-01
Gly-Gly	Amine	-0.0116	0.3095	-0.0376	9.7004E-01	9.9011E-01
5-OH-Trp	Amine	0.0189	0.7545	0.0251	9.7998E-01	9.9348E-01
Glutathione	Amine	-0.0072	0.3321	-0.0216	9.8275E-01	9.9348E-01
LPE (22:5)	Lysophospholipid	0.0143	0.7564	0.0189	9.8488E-01	9.9348E-01
LPI (20:4)	Lysophospholipid	-0.0094	0.7197	-0.0131	9.8956E-01	9.9348E-01
Ala	Amine	-0.0166	1.3428	-0.0124	9.9012E-01	9.9348E-01
10-HDoHE/DHA	Oxylipin	0.0014	0.4081	0.0035	9.9723E-01	9.9723E-01

Table S13: Logistic regression results of the "SINS_S" model comparing systemic inflammation-no sepsis with sepsis in the single time point dataset

Metabolite	Category	Estimate	Standard Error	z-value	p-value	Adjusted p-value
BCAA/AAA	Amine	3.9450	1.6041	2.4593	1.3921E-02	8.5266E-01
LPS (20:4)	Lysophospholipid	-2.3189	1.0040	-2.3095	2.0914E-02	8.5266E-01
LPE (20:4)	Lysophospholipid	-3.5010	1.5294	-2.2892	2.2069E-02	8.5266E-01
12,13-EpOME/LA	Oxylipin	-1.5415	0.7084	-2.1760	2.9553E-02	8.5266E-01
Sum BA	Bile Acid	0.4254	0.1961	2.1692	3.0064E-02	8.5266E-01
11beta-PGF2alpha/AA	Oxylipin	0.9061	0.4202	2.1564	3.1052E-02	8.5266E-01
Putrescine	Amine	1.6002	0.7426	2.1550	3.1162E-02	8.5266E-01
LPA (20:3)	Lysophospholipid	-1.7805	0.8289	-2.1480	3.1715E-02	8.5266E-01
BCAA/Tyr	Amine	2.2764	1.1051	2.0598	3.9413E-02	8.5266E-01
LPA (20:4)	Lysophospholipid	-1.6955	0.8262	-2.0522	4.0155E-02	8.5266E-01
Mead.AcId	Fatty acid	-1.0741	0.5264	-2.0406	4.1286E-02	8.5266E-01
LPS (18:1)	Lysophospholipid	-1.2820	0.6327	-2.0263	4.2739E-02	8.5266E-01
SIP (18:2)	Lysophospholipid	-2.4143	1.2140	-1.9887	4.6735E-02	8.5266E-01
Cortisol	Steroid Hormone	1.0755	0.5459	1.9702	4.8817E-02	8.5266E-01

Chapter III

11beta-PGF2alpha	Oxylipin	0.8757	0.4481	1.9543	5.0668E-02	8.5266E-01
LPA (22:4)	Lysophospholipid	-1.0811	0.5682	-1.9026	5.7088E-02	8.5266E-01
LPA (18:1)	Lysophospholipid	-1.4269	0.7719	-1.8487	6.4501E-02	8.5266E-01
3-Methoxy-tyrosine	Amine	-1.2289	0.6654	-1.8469	6.4767E-02	8.5266E-01
LPI (16:0)	Lysophospholipid	1.7655	0.9670	1.8257	6.7889E-02	8.5266E-01
SIP (18:0)	Lysophospholipid	-1.2058	0.6701	-1.7994	7.1952E-02	8.5266E-01
SIP (18:1)	Lysophospholipid	-1.8364	1.0210	-1.7986	7.2085E-02	8.5266E-01
5-HETrE	Oxylipin	-1.0639	0.5938	-1.7917	7.3182E-02	8.5266E-01
Sum SBA	Bile Acid	1.7174	0.9672	1.7757	7.5783E-02	8.5266E-01
8-iso-PGF3alpha	Oxylipin	0.4409	0.2624	1.6801	9.2944E-02	8.5266E-01
cLPA (18:1)	Lysophospholipid	-0.7729	0.4609	-1.6770	9.3548E-02	8.5266E-01
LPA (16:0)	Lysophospholipid	-1.0897	0.6536	-1.6672	9.5484E-02	8.5266E-01
ADMA	Amine	-1.5269	0.9312	-1.6397	1.0108E-01	8.5266E-01
LPA (22:6)	Lysophospholipid	-1.2102	0.7383	-1.6392	1.0118E-01	8.5266E-01
5-HETrE/DGLA	Oxylipin	-0.6951	0.4243	-1.6382	1.0137E-01	8.5266E-01
LPE (18:1)	Lysophospholipid	-1.7059	1.0432	-1.6352	1.0201E-01	8.5266E-01
PGE2	Oxylipin	-0.5352	0.3275	-1.6343	1.0219E-01	8.5266E-01
FA (18:0)	Fatty acid	-1.1695	0.7333	-1.5948	1.1076E-01	8.5266E-01
Sum HETEs	Oxylipin	-1.0319	0.6472	-1.5943	1.1086E-01	8.5266E-01
Tau	Amine	-1.2240	0.7826	-1.5641	1.1779E-01	8.5266E-01
LPA (16:1)	Lysophospholipid	-0.8275	0.5457	-1.5164	1.2942E-01	8.5266E-01
12,13-DiHOME/12,13-EpOME	Oxylipin	1.0519	0.6964	1.5105	1.3091E-01	8.5266E-01
Met-SO	Amine	-1.7613	1.1667	-1.5096	1.3114E-01	8.5266E-01
AAA	Amine	-1.5745	1.0431	-1.5094	1.3119E-01	8.5266E-01
3-Met-His	Amine	-1.1733	0.7845	-1.4956	1.3477E-01	8.5266E-01
cLPA (20:4)	Lysophospholipid	-0.7528	0.5045	-1.4922	1.3565E-01	8.5266E-01
8-iso-PGF3alpha/DGLA	Oxylipin	0.3486	0.2343	1.4881	1.3673E-01	8.5266E-01
2,3-dinor-8-iso-PGF2alpha/AA	Oxylipin	0.7690	0.5301	1.4508	1.4682E-01	8.5266E-01
9-HEPE/EPA	Oxylipin	-0.9993	0.6888	-1.4508	1.4682E-01	8.5266E-01
LPS (22:6)	Lysophospholipid	-1.0324	0.7127	-1.4485	1.4748E-01	8.5266E-01
12-HETE	Oxylipin	-0.4745	0.3298	-1.4389	1.5018E-01	8.5266E-01
Tyr	Amine	-1.0193	0.7140	-1.4276	1.5342E-01	8.5266E-01
Thr	Amine	-1.0863	0.7621	-1.4255	1.5402E-01	8.5266E-01
LPI (18:0)	Lysophospholipid	1.4657	1.0292	1.4241	1.5443E-01	8.5266E-01
OH-Lys/Lys	Amine	-1.2486	0.8920	-1.3998	1.6158E-01	8.5266E-01
DHEA	Endocannabinoid	0.9886	0.7086	1.3952	1.6294E-01	8.5266E-01
AABA	Amine	0.6964	0.5036	1.3830	1.6666E-01	8.5266E-01
TLCA-3S	Bile Acid	0.3600	0.2629	1.3694	1.7088E-01	8.5266E-01
Arg/Lys	Amine	-1.2560	0.9198	-1.3656	1.7207E-01	8.5266E-01
8,12-iso-iPF2alpha-VI	Oxylipin	-1.0924	0.8030	-1.3604	1.7370E-01	8.5266E-01
20-HETE	Oxylipin	-1.1671	0.8584	-1.3597	1.7392E-01	8.5266E-01
OA	Fatty acid	-2.7224	2.0255	-1.3441	1.7893E-01	8.5266E-01
PAF 18(2)	PAF	0.3537	0.2644	1.3378	1.8098E-01	8.5266E-01
12,13-EpOME	Oxylipin	-0.7219	0.5412	-1.3341	1.8218E-01	8.5266E-01
10-HDoHE/DHA	Oxylipin	-0.6557	0.4976	-1.3178	1.8757E-01	8.5266E-01
13,14-dihydro-15-keto-PGF2alpha	Oxylipin	-0.5611	0.4264	-1.3160	1.8817E-01	8.5266E-01
Phe/Tyr	Amine	1.0661	0.8134	1.3107	1.8997E-01	8.5266E-01
FA (16:0)	Fatty acid	-0.8634	0.6614	-1.3054	1.9177E-01	8.5266E-01
5-HETE	Oxylipin	-1.0512	0.8076	-1.3016	1.9304E-01	8.5266E-01
Sarcosine	Amine	0.5802	0.4460	1.3007	1.9335E-01	8.5266E-01
5-KETE/5-HETE	Oxylipin	0.9239	0.7170	1.2886	1.9754E-01	8.5266E-01
LPE (18:0)	Lysophospholipid	1.1880	0.9223	1.2881	1.9770E-01	8.5266E-01
10-HDoHE	Oxylipin	-0.4919	0.3821	-1.2871	1.9805E-01	8.5266E-01
Cys	Amine	0.8924	0.6991	1.2764	2.0183E-01	8.5266E-01
12-HHTrE	Oxylipin	-0.5326	0.4181	-1.2738	2.0273E-01	8.5266E-01
14-HDoHE	Oxylipin	-0.3598	0.2869	-1.2542	2.0977E-01	8.5266E-01
12-KETE/12-HETE	Oxylipin	0.4944	0.3950	1.2516	2.1071E-01	8.5266E-01
Citrulline	Amine	-0.9787	0.7829	-1.2500	2.1131E-01	8.5266E-01
14-HDoHE/DHA	Oxylipin	-0.4126	0.3322	-1.2422	2.1415E-01	8.5266E-01
4-OH-Pro/Pro	Amine	-1.0135	0.8284	-1.2235	2.2115E-01	8.5266E-01
Sum HDoHEs	Oxylipin	-0.4176	0.3442	-1.2132	2.2505E-01	8.5266E-01
LPE (22:5)	Lysophospholipid	1.0904	0.9036	1.2067	2.2756E-01	8.5266E-01
LPI (14:0)	Lysophospholipid	0.8680	0.7277	1.1928	2.3294E-01	8.5266E-01
PGE2/AA	Oxylipin	-0.4561	0.3837	-1.1889	2.3446E-01	8.5266E-01
12-HETE/AA	Oxylipin	-0.4594	0.3886	-1.1821	2.3718E-01	8.5266E-01
LPA (14:0)	Lysophospholipid	-0.6763	0.5791	-1.1680	2.4283E-01	8.5266E-01
HomoCys	Amine	0.7128	0.6156	1.1579	2.4689E-01	8.5266E-01
PGF2alpha	Oxylipin	-0.4257	0.3692	-1.1532	2.4885E-01	8.5266E-01
8-HETrE/DGLA	Oxylipin	-0.5285	0.4599	-1.1493	2.5044E-01	8.5266E-01
Sum HEPEs	Oxylipin	-0.3816	0.3333	-1.1451	2.5217E-01	8.5266E-01
delta-17,6-keto-PGF1alpha/EPA	Oxylipin	-0.2563	0.2242	-1.1433	2.5293E-01	8.5266E-01
OH-Lys	Amine	-1.0504	0.9190	-1.1430	2.5303E-01	8.5266E-01
LPG (18:1)	Lysophospholipid	-1.3806	1.2215	-1.1302	2.5838E-01	8.5266E-01
LPS (16:0)	Lysophospholipid	2.8703	2.5509	1.1252	2.6051E-01	8.5266E-01

Diagnosis of Late-Onset Sepsis

LA	Fatty acid	0.9315	0.8335	1.1176	2.6373E-01	8.5266E-01
LPI (18:2)	Lysophospholipid	0.8466	0.7583	1.1165	2.6421E-01	8.5266E-01
LPE (16:0)	Lysophospholipid	0.8927	0.8035	1.1110	2.6657E-01	8.5266E-01
O-Acetyl-Ser	Amine	0.7268	0.6546	1.1102	2.6693E-01	8.5266E-01
5-OH-Trp	Amine	-0.9321	0.8639	-1.0789	2.8063E-01	8.5266E-01
CA	Bile Acid	-0.2466	0.2287	-1.0785	2.8081E-01	8.5266E-01
LPA (18:2)	Lysophospholipid	-0.6785	0.6302	-1.0767	2.8161E-01	8.5266E-01
18-HEPE/EPA	Oxylipin	-0.5068	0.4770	-1.0625	2.8800E-01	8.5266E-01
GABA	Amine	0.7897	0.7461	1.0584	2.8988E-01	8.5266E-01
Val	Amine	1.2938	1.2330	1.0493	2.9405E-01	8.5266E-01
AA	Fatty acid	-0.7479	0.7261	-1.0299	3.0304E-01	8.5266E-01
Carnosine	Amine	-0.5410	0.5263	-1.0280	3.0395E-01	8.5266E-01
Sum LG	Endocannabinoid	0.4562	0.4453	1.0245	3.0559E-01	8.5266E-01
ETE	Fatty acid	-0.6868	0.6719	-1.0223	3.0665E-01	8.5266E-01
Glu/GABA	Amine	-0.7048	0.6979	-1.0098	3.1261E-01	8.5266E-01
Kyn	Amine	-0.4472	0.4430	-1.0096	3.1270E-01	8.5266E-01
LPE (16:1)	Lysophospholipid	-0.6558	0.6562	-0.9994	3.1762E-01	8.5266E-01
LPE (22:6)	Lysophospholipid	-1.1065	1.1087	-0.9981	3.1824E-01	8.5266E-01
DPA	Fatty acid	-0.4613	0.4623	-0.9978	3.1836E-01	8.5266E-01
9-HpODE/LA	Oxylipin	-0.5186	0.5242	-0.9894	3.2245E-01	8.5266E-01
Met-SO2	Amine	-0.6998	0.7096	-0.9862	3.2405E-01	8.5266E-01
Pro	Amine	1.1326	1.1601	0.9763	3.2893E-01	8.5266E-01
Arg	Amine	-0.6864	0.7189	-0.9547	3.3974E-01	8.5266E-01
LPS (18:0)	Lysophospholipid	-0.4949	0.5197	-0.9524	3.4091E-01	8.5266E-01
LPE (20:3)	Lysophospholipid	-0.8459	0.8887	-0.9519	3.4113E-01	8.5266E-01
Phe	Amine	-1.0508	1.1078	-0.9486	3.4283E-01	8.5266E-01
Sum HETrEs	Oxylipin	-0.4200	0.4475	-0.9385	3.4801E-01	8.5266E-01
8-HETrE	Oxylipin	-0.3776	0.4048	-0.9327	3.5097E-01	8.5266E-01
LPG (20:4)	Lysophospholipid	-0.9593	1.0359	-0.9261	3.5441E-01	8.5266E-01
Homocitrulline	Amine	-0.6669	0.7236	-0.9216	3.5673E-01	8.5266E-01
Gly-Gly	Amine	-0.3580	0.3894	-0.9191	3.5803E-01	8.5266E-01
14,15-DiHETrE	Oxylipin	-0.6331	0.6890	-0.9189	3.5816E-01	8.5266E-01
Sum PGs	Oxylipin	-0.3149	0.3445	-0.9141	3.6065E-01	8.5266E-01
PGA2	Oxylipin	-0.4289	0.4693	-0.9140	3.6071E-01	8.5266E-01
LPI (16:1)	Lysophospholipid	0.6218	0.6849	0.9079	3.6393E-01	8.5266E-01
LPA (20:5)	Lysophospholipid	-0.5505	0.6092	-0.9036	3.6618E-01	8.5266E-01
19,20-EpDPE/DHA	Oxylipin	0.4971	0.5527	0.8994	3.6842E-01	8.5266E-01
5-HEPE/EPA	Oxylipin	-0.6186	0.6900	-0.8965	3.6997E-01	8.5266E-01
12-HHTrE/AA	Oxylipin	-0.3776	0.4259	-0.8866	3.7527E-01	8.5266E-01
BCAA	Amine	1.1240	1.2712	0.8842	3.7661E-01	8.5266E-01
17-HDoHE	Oxylipin	-0.3383	0.3893	-0.8690	3.8483E-01	8.5266E-01
Asp	Amine	-0.5985	0.6894	-0.8681	3.8532E-01	8.5266E-01
9-HEPE	Oxylipin	-0.3359	0.3877	-0.8663	3.8632E-01	8.5266E-01
TUDCA	Bile Acid	0.2285	0.2667	0.8569	3.9150E-01	8.5266E-01
12-HEPE/EPA	Oxylipin	-0.3059	0.3571	-0.8565	3.9174E-01	8.5266E-01
LPE (18:3)	Lysophospholipid	-0.3674	0.4298	-0.8548	3.9267E-01	8.5266E-01
15-HEPE/EPA	Oxylipin	-0.4767	0.5592	-0.8525	3.9392E-01	8.5266E-01
LPI (22:6)	Lysophospholipid	0.8349	0.9805	0.8515	3.9450E-01	8.5266E-01
17-HDoHE/DHA	Oxylipin	-0.4588	0.5390	-0.8512	3.9465E-01	8.5266E-01
Sphinganine 18.0	Lysophospholipid	0.5135	0.6107	0.8409	4.0042E-01	8.5727E-01
11-HETE	Oxylipin	-0.4358	0.5252	-0.8297	4.0670E-01	8.5727E-01
Ornithine	Amine	-0.6067	0.7364	-0.8238	4.1005E-01	8.5727E-01
cLPA (18:2)	Lysophospholipid	-0.3293	0.3999	-0.8235	4.1021E-01	8.5727E-01
LPA (18:0)	Lysophospholipid	-0.5684	0.6917	-0.8217	4.1126E-01	8.5727E-01
1-Met-His	Amine	-1.9329	2.3693	-0.8158	4.1461E-01	8.5822E-01
11-HDoHE	Oxylipin	-0.2775	0.3428	-0.8094	4.1829E-01	8.5978E-01
11,12-DiHETrE	Oxylipin	-0.4775	0.5947	-0.8030	4.2196E-01	8.5978E-01
Trp	Amine	-0.9703	1.2138	-0.7994	4.2408E-01	8.5978E-01
5-HEPE	Oxylipin	-0.4712	0.6016	-0.7831	4.3355E-01	8.7000E-01
Kyn/Trp	Amine	-0.3686	0.4771	-0.7726	4.3976E-01	8.7000E-01
LPG (22:4)	Lysophospholipid	-0.6886	0.8972	-0.7675	4.4279E-01	8.7000E-01
Sphingosine 18.1	Lysophospholipid	0.4323	0.5697	0.7589	4.4793E-01	8.7000E-01
LPE (14:0)	Lysophospholipid	0.4812	0.6347	0.7582	4.4835E-01	8.7000E-01
LPG (18:3)	Lysophospholipid	-0.4856	0.6411	-0.7575	4.4872E-01	8.7000E-01
20-HDoHE	Oxylipin	-0.3681	0.4875	-0.7550	4.5028E-01	8.7000E-01
w3FA/w6FA	Fatty acid	0.5355	0.7130	0.7510	4.5263E-01	8.7000E-01
LPA (22:5)	Lysophospholipid	-0.4288	0.5886	-0.7285	4.6634E-01	8.9055E-01
11-HDoHE/DHA	Oxylipin	-0.2910	0.4037	-0.7209	4.7097E-01	8.9225E-01
2,3-dinor-8-iso-PGF2alpha	Oxylipin	0.3248	0.4531	0.7168	4.7352E-01	8.9225E-01
15-HETE	Oxylipin	-0.3074	0.4375	-0.7026	4.8227E-01	8.9225E-01
GCA	Bile Acid	0.1174	0.1674	0.7013	4.8311E-01	8.9225E-01
THDCA	Bile Acid	-0.1920	0.2754	-0.6970	4.8578E-01	8.9225E-01
Ile	Amine	0.8214	1.1849	0.6933	4.8813E-01	8.9225E-01
12-HEPE	Oxylipin	-0.1958	0.2826	-0.6930	4.8832E-01	8.9225E-01

Chapter III

18-HEPE	Oxylipin	-0.2718	0.4008	-0.6783	4.9761E-01	9.0006E-01
LPI (18:1)	Lysophospholipid	0.6564	0.9800	0.6698	5.0300E-01	9.0006E-01
Sum TXs	Oxylipin	-0.2355	0.3537	-0.6658	5.0554E-01	9.0006E-01
LPS (18:2)	Lysophospholipid	-0.4138	0.6243	-0.6629	5.0738E-01	9.0006E-01
PGF2alpha/AA	Oxylipin	-0.2431	0.3695	-0.6578	5.1066E-01	9.0006E-01
15-HEPE	Oxylipin	-0.2679	0.4074	-0.6575	5.1085E-01	9.0006E-01
TCA	Bile Acid	0.1480	0.2332	0.6346	5.2566E-01	9.0636E-01
13,14-dihydro-15-keto-PGF2alpha/AA	Oxylipin	-0.2641	0.4175	-0.6325	5.2705E-01	9.0636E-01
5-IPF2alpha-VI	Oxylipin	-0.4843	0.7674	-0.6311	5.2798E-01	9.0636E-01
delta-17,6-keto-PGF1alpha	Oxylipin	-0.1471	0.2342	-0.6279	5.3006E-01	9.0636E-01
Homoserine	Amine	-0.5152	0.8297	-0.6209	5.3465E-01	9.0636E-01
Trimethyl-Lys	Amine	0.6036	0.9741	0.6196	5.3550E-01	9.0636E-01
PGF1alpha/DGLA	Oxylipin	0.1356	0.2193	0.6182	5.3643E-01	9.0636E-01
LPI (20:4)	Lysophospholipid	0.7298	1.1939	0.6113	5.4098E-01	9.0636E-01
SIP (16:1)	Lysophospholipid	-0.4811	0.7889	-0.6098	5.4198E-01	9.0636E-01
14,15-DiHETE	Oxylipin	0.2887	0.5080	0.5683	5.6986E-01	9.4763E-01
9-KODE	Oxylipin	0.2945	0.5241	0.5619	5.7416E-01	9.4899E-01
TXB3/EPA	Oxylipin	-0.1610	0.2957	-0.5445	5.8608E-01	9.4899E-01
GCDA	Bile Acid	0.0926	0.1704	0.5434	5.8684E-01	9.4899E-01
Leu	Amine	0.7410	1.3786	0.5375	5.9092E-01	9.4899E-01
7-HDoHE	Oxylipin	-0.2348	0.4383	-0.5355	5.9227E-01	9.4899E-01
20-HDoHE/DHA	Oxylipin	-0.3146	0.5886	-0.5344	5.9305E-01	9.4899E-01
LPE (22:4)	Lysophospholipid	-0.3585	0.6800	-0.5273	5.9800E-01	9.4899E-01
cLPA (16:1)	Lysophospholipid	-0.4084	0.7772	-0.5255	5.9927E-01	9.4899E-01
11,12-EpETrE/AA	Oxylipin	0.3101	0.5929	0.5230	6.0100E-01	9.4899E-01
TXB3/EPA	Oxylipin	-0.1453	0.2816	-0.5157	6.0605E-01	9.4899E-01
g-Glu-Gln	Amine	0.1898	0.3689	0.5145	6.0694E-01	9.4899E-01
4-OH-Pro	Amine	-0.3984	0.7816	-0.5098	6.1022E-01	9.4899E-01
LPE (18:2)	Lysophospholipid	-0.3377	0.6788	-0.4975	6.1880E-01	9.4899E-01
19,20-EpDPE	Oxylipin	0.2453	0.4940	0.4965	6.1954E-01	9.4899E-01
17,18-DiHETE	Oxylipin	0.1704	0.3436	0.4959	6.1997E-01	9.4899E-01
PGE1	Oxylipin	0.1602	0.3282	0.4881	6.2550E-01	9.4899E-01
Citrulline/Ornithine	Amine	-0.3672	0.7690	-0.4776	6.3296E-01	9.4899E-01
Sum OG	Endocannabinoid	-0.2415	0.5180	-0.4662	6.4104E-01	9.4899E-01
TXB2	Oxylipin	-0.1551	0.3345	-0.4637	6.4286E-01	9.4899E-01
15-HETE/DGLA	Oxylipin	-0.2215	0.4784	-0.4631	6.4330E-01	9.4899E-01
Cystathionine	Amine	0.1901	0.4106	0.4629	6.4345E-01	9.4899E-01
Lys	Amine	0.4817	1.0416	0.4625	6.4374E-01	9.4899E-01
Ala	Amine	0.5843	1.2665	0.4614	6.4455E-01	9.4899E-01
13-HDoHE	Oxylipin	-0.2027	0.4464	-0.4540	6.4981E-01	9.4899E-01
Gly	Amine	-0.5231	1.1608	-0.4506	6.5225E-01	9.4899E-01
Arg/ADMA	Amine	0.2912	0.6498	0.4482	6.5404E-01	9.4899E-01
5-HT/Trp	Amine	0.1145	0.2613	0.4380	6.6139E-01	9.4991E-01
LPG (14:0)	Lysophospholipid	0.2940	0.6751	0.4354	6.6325E-01	9.4991E-01
9-HOTrE	Oxylipin	-0.1765	0.4081	-0.4325	6.6537E-01	9.4991E-01
3-Methoxy-tyramine	Amine	-0.5044	1.1743	-0.4296	6.6750E-01	9.4991E-01
Saccharopine	Amine	0.1602	0.3825	0.4188	6.7539E-01	9.5644E-01
19,20-DiHDPA/19,20-EpDPE	Oxylipin	-0.1896	0.4640	-0.4086	6.8280E-01	9.5644E-01
Cys/Cystathionine	Amine	0.1503	0.3813	0.3940	6.9357E-01	9.5644E-01
cLPA (18:0)	Lysophospholipid	-0.2197	0.5593	-0.3928	6.9445E-01	9.5644E-01
Glutathione	Amine	-0.1588	0.4046	-0.3924	6.9480E-01	9.5644E-01
Gly-Pro	Amine	-0.2268	0.5879	-0.3858	6.9966E-01	9.5644E-01
LPG (16:1)	Lysophospholipid	-0.2517	0.6644	-0.3788	7.0483E-01	9.5644E-01
Sum PBA	Bile Acid	0.0734	0.1965	0.3734	7.0882E-01	9.5644E-01
Cystathionine/HomoCys	Amine	-0.1433	0.3897	-0.3679	7.1298E-01	9.5644E-01
11,12-EpTrE	Oxylipin	-0.2140	0.5972	-0.3583	7.2011E-01	9.5644E-01
8-HDoHE/DHA	Oxylipin	0.2188	0.6143	0.3561	7.2175E-01	9.5644E-01
Sum AG	Endocannabinoid	0.1346	0.3783	0.3559	7.2193E-01	9.5644E-01
11,12-DiHETrE/11,12-EpETrE	Oxylipin	-0.1571	0.4424	-0.3552	7.2245E-01	9.5644E-01
beta-Ala	Amine	0.3669	1.0358	0.3542	7.2319E-01	9.5644E-01
9-HOTrE/ALA	Oxylipin	-0.1705	0.4936	-0.3455	7.2970E-01	9.5644E-01
Ser	Amine	-0.3236	0.9741	-0.3321	7.3978E-01	9.5644E-01
O-PO3-EA	Amine	-0.1347	0.4130	-0.3262	7.4426E-01	9.5644E-01
LPG (16:0)	Lysophospholipid	0.3156	0.9712	0.3249	7.4524E-01	9.5644E-01
5-aminolevulinic acid	Amine	-0.1961	0.6097	-0.3216	7.4772E-01	9.5644E-01
LPE (20:5)	Lysophospholipid	-0.3815	1.2014	-0.3176	7.5082E-01	9.5644E-01
Sum DiHETrEs	Oxylipin	-0.2115	0.6666	-0.3172	7.5107E-01	9.5644E-01
PGF1alpha	Oxylipin	0.0778	0.2453	0.3172	7.5111E-01	9.5644E-01
7-HDoHE/DHA	Oxylipin	-0.1659	0.5365	-0.3092	7.5719E-01	9.5644E-01
DHA	Fatty acid	-0.1463	0.4778	-0.3062	7.5943E-01	9.5644E-01
HCA	Bile Acid	-0.0591	0.1957	-0.3018	7.6282E-01	9.5644E-01
8,9-DiHETrE	Oxylipin	0.1517	0.5143	0.2951	7.6795E-01	9.5644E-01
9-KODE/9-HODE	Oxylipin	0.2143	0.7300	0.2936	7.6904E-01	9.5644E-01
15-HETrE	Oxylipin	-0.1292	0.4402	-0.2934	7.6920E-01	9.5644E-01

Diagnosis of Late-Onset Sepsis

9-HODE	Oxylipin	0.1262	0.4351	0.2901	7.7174E-01	9.5644E-01
ADA	Fatty acid	-0.1455	0.5074	-0.2868	7.7428E-01	9.5644E-01
LCA	Bile Acid	0.3414	1.2111	0.2819	7.7801E-01	9.5644E-01
8,12-iso-iPF2alpha-VI/AA	Oxylipin	-0.2075	0.7364	-0.2818	7.7813E-01	9.5644E-01
16-HDoHE/DHA	Oxylipin	0.1732	0.6252	0.2770	7.8181E-01	9.5644E-01
5-KETE	Oxylipin	0.2462	0.8895	0.2768	7.8196E-01	9.5644E-01
5-HETE/AA	Oxylipin	-0.1991	0.7639	-0.2606	7.9437E-01	9.5924E-01
5-HT	Amine	0.0625	0.2492	0.2508	8.0196E-01	9.5924E-01
LPI (22:4)	Lysophospholipid	-0.2447	0.9807	-0.2495	8.0299E-01	9.5924E-01
Sum iPs	Oxylipin	0.0609	0.2472	0.2463	8.0547E-01	9.5924E-01
9-HpODE	Oxylipin	-0.1200	0.5011	-0.2396	8.1068E-01	9.5924E-01
DEA	Endocannabinoid	0.1586	0.6628	0.2392	8.1092E-01	9.5924E-01
SDMA	Amine	-0.2115	0.8849	-0.2391	8.1106E-01	9.5924E-01
LPG (22:6)	Lysophospholipid	-0.1404	0.6020	-0.2332	8.1558E-01	9.5924E-01
cLPA (14:0)	Lysophospholipid	0.1444	0.6250	0.2310	8.1735E-01	9.5924E-01
13-HDoHE/DHA	Oxylipin	-0.1323	0.5854	-0.2259	8.2126E-01	9.5924E-01
12-KETE	Oxylipin	0.0579	0.2601	0.2225	8.2394E-01	9.5924E-01
TXBI/DGLA	Oxylipin	-0.0804	0.3623	-0.2218	8.2450E-01	9.5924E-01
ALA	Fatty acid	-0.1255	0.5934	-0.2114	8.3255E-01	9.5924E-01
20-HETE/AA	Oxylipin	-0.1663	0.7923	-0.2099	8.3372E-01	9.5924E-01
LPG (18:2)	Lysophospholipid	-0.1177	0.5892	-0.1997	8.4171E-01	9.5924E-01
Ornithine/Arg	Amine	0.1157	0.5798	0.1995	8.4191E-01	9.5924E-01
2-aminoadipic acid	Amine	0.1073	0.5482	0.1958	8.4479E-01	9.5924E-01
Asn	Amine	-0.1411	0.7232	-0.1951	8.4529E-01	9.5924E-01
Gln	Amine	0.1185	0.6094	0.1945	8.4581E-01	9.5924E-01
12,13-DiHOME	Oxylipin	-0.1065	0.5640	-0.1888	8.5027E-01	9.6061E-01
Anserine	Amine	0.0820	0.4478	0.1832	8.5465E-01	9.6189E-01
Gln/Glu	Amine	0.0761	0.4486	0.1696	8.6533E-01	9.6424E-01
GLA	Fatty acid	0.1347	0.8136	0.1656	8.6851E-01	9.6424E-01
LPG (20:3)	Lysophospholipid	-0.1610	1.0180	-0.1581	8.7434E-01	9.6424E-01
Sum HODEs	Oxylipin	0.0685	0.4381	0.1563	8.7577E-01	9.6424E-01
PGA2/AA	Oxylipin	-0.0799	0.5136	-0.1556	8.7637E-01	9.6424E-01
DGLA	Fatty acid	0.0747	0.4847	0.1541	8.7751E-01	9.6424E-01
Clupanodonic acid	Fatty acid	0.0588	0.3901	0.1506	8.8026E-01	9.6424E-01
5,6-DiHETE	Oxylipin	-0.0587	0.3979	-0.1474	8.8280E-01	9.6424E-01
LPS (22:4)	Lysophospholipid	-0.1092	0.8809	-0.1240	9.0130E-01	9.7985E-01
AEA	Endocannabinoid	-0.0881	0.7280	-0.1210	9.0371E-01	9.7985E-01
5-iPF2alpha-VI/AA	Oxylipin	0.0691	0.6078	0.1136	9.0954E-01	9.8257E-01
S-Methyl-Cys	Amine	0.0974	0.9281	0.1049	9.1643E-01	9.8526E-01
11-HETE/AA	Oxylipin	-0.0688	0.6742	-0.1021	9.1869E-01	9.8526E-01
16-HDoHE	Oxylipin	-0.0439	0.4680	-0.0937	9.2534E-01	9.8881E-01
Sum KETEs	Oxylipin	-0.0291	0.3517	-0.0828	9.3398E-01	9.8926E-01
15-HETE/AA	Oxylipin	-0.0481	0.5901	-0.0815	9.3501E-01	9.8926E-01
EA	Amine	0.0563	0.7037	0.0800	9.3620E-01	9.8926E-01
TXBI	Oxylipin	0.0316	0.4271	0.0741	9.4093E-01	9.8926E-01
Met	Amine	-0.0682	0.9455	-0.0722	9.4247E-01	9.8926E-01
Sum DiHETEs	Oxylipin	-0.0280	0.4132	-0.0677	9.4599E-01	9.8944E-01
19,20-DiHDPA	Oxylipin	0.0252	0.4480	0.0562	9.5517E-01	9.9364E-01
Glu	Amine	-0.0483	0.9124	-0.0529	9.5782E-01	9.9364E-01
His	Amine	-0.0546	1.0910	-0.0501	9.6007E-01	9.9364E-01
PGE1/DGLA	Oxylipin	-0.1019	0.3312	-0.0329	9.7373E-01	9.9837E-01
g-Glu-Ala	Amine	0.0122	0.3939	0.0309	9.7533E-01	9.9837E-01
8-HDoHE	Oxylipin	-0.0111	0.4477	-0.0248	9.8021E-01	9.9837E-01
TXB2/AA	Oxylipin	0.0074	0.3249	0.0229	9.8173E-01	9.9837E-01
3-AIBA	Amine	0.0065	0.3554	0.0182	9.8549E-01	9.9837E-01
9-HODE/9-HpODE	Oxylipin	0.0094	0.5413	0.0175	9.8608E-01	9.9837E-01
LPG (18:0)	Lysophospholipid	0.0061	0.7890	0.0077	9.9386E-01	9.9837E-01
Coriolic acid	Oxylipin	0.0033	0.4304	0.0077	9.9388E-01	9.9837E-01
PAF 16(0)	PAF	0.0021	0.4737	0.0045	9.9643E-01	9.9837E-01
EPA	Fatty acid	0.0008	0.4152	0.0020	9.9837E-01	9.9837E-01

Table S14: Performance metrics of multivariable metabolomic models across 100 bootstrap iterations

Iteration	AUC	Sensitivity	Specificity
1	0.7456	0.8947	0.6667
2	0.5286	0.2000	1.0000
3	0.5648	0.4167	0.8889
4	0.7041	0.7143	0.8571
5	0.5375	0.6875	0.6000
6	0.6190	0.5333	0.8571
7	0.6083	0.5333	0.7500
8	0.7895	0.8421	0.8000
9	0.4904	0.3846	0.8750

Chapter III

10	0.6094	0.5625	0.7500
11	0.8182	0.8182	0.7500
12	0.6548	0.8571	0.5000
13	0.7333	0.8667	0.6667
14	0.5510	0.6429	0.5714
15	0.4667	0.4000	0.8333
16	0.4800	0.9333	0.2000
17	0.6125	0.7500	0.6000
18	0.6000	0.5385	0.8000
19	0.4952	1.0000	0.1429
20	0.5926	0.3333	1.0000
21	0.5253	0.8182	0.4444
22	0.5317	0.5556	0.7143
23	0.5446	0.5625	0.7143
24	0.5000	1.0000	0.0000
25	0.7238	0.6667	0.8000
26	0.5408	0.2857	1.0000
27	0.6296	0.7500	0.5556
28	0.5222	0.5333	0.6667
29	0.5556	0.9333	0.3333
30	0.5833	1.0000	0.3333
31	0.5897	0.6923	0.6667
32	0.4412	1.0000	0.1667
33	0.6235	0.3529	1.0000
34	0.6250	0.6667	0.7500
35	0.5357	0.8571	0.3333
36	0.6964	0.9375	0.5714
37	0.5960	0.7273	0.6667
38	0.7857	0.8571	0.7143
39	0.5897	0.6923	0.5556
40	0.6800	0.5333	1.0000
41	0.7031	0.7500	0.7500
42	0.5889	0.4667	0.8333
43	0.6538	0.3846	1.0000
44	0.4872	0.3077	1.0000
45	0.4583	0.6667	0.5000
46	0.7193	0.6316	1.0000
47	0.6000	0.7059	0.6000
48	0.5500	0.7333	0.5000
49	0.5048	0.4000	0.8571
50	0.7111	0.5556	1.0000
51	0.6471	0.7647	0.6667
52	0.5824	0.5385	0.8571
53	0.7206	0.5294	1.0000
54	0.5000	0.8667	0.5000
55	0.6667	0.6000	0.8571
56	0.9333	0.8667	1.0000
57	0.6500	1.0000	0.4000
58	0.6250	0.7857	0.6250
59	0.5317	0.7222	0.4286
60	0.5515	0.8235	0.5000
61	0.5210	0.7647	0.5714
62	0.5204	0.5000	0.7143
63	0.4667	0.5333	0.6000
64	0.6154	0.7692	0.5000
65	0.5583	0.2667	1.0000
66	0.5000	1.0000	0.0000
67	0.4583	1.0000	0.1667
68	0.5500	0.8333	0.5000
69	0.5600	0.6000	0.8000
70	0.6857	1.0000	0.4000
71	0.7857	0.5625	1.0000
72	0.5882	0.7059	0.6000
73	0.7200	0.9333	0.6000
74	0.4808	0.6154	0.5000
75	0.5965	0.3158	1.0000
76	0.7917	0.6667	1.0000
77	0.7222	0.9444	0.5000
78	0.5486	0.4375	0.8889
79	0.5982	0.4375	0.8571
80	0.5741	0.6667	0.5556
81	0.4800	0.8000	0.4000
82	0.5882	0.6471	0.7500
83	0.5903	0.4375	0.8889

84	0.6373	0.5882	0.8333
85	0.5179	0.8125	0.4286
86	0.6688	0.9286	0.4545
87	0.5357	0.5000	0.7143
88	0.5867	0.7333	0.6000
89	0.5952	0.9167	0.5714
90	0.7353	0.5294	1.0000
91	0.8462	0.6923	1.0000
92	0.7698	0.7143	0.7778
93	0.6806	0.5833	0.8333
94	0.6286	0.7857	0.6000
95	0.6316	0.6316	0.7500
96	0.4000	1.0000	0.0000
97	0.5600	0.9000	0.6000
98	0.5096	0.8462	0.3750
99	0.6807	0.9412	0.4286
100	0.7083	0.8667	0.6250

Table S15: Model parameters of diagnostic models to differentiate between systemic inflammation-no sepsis and sepsis at the moment of suspicion

Model	AUC	Threshold	Sensitivity	Specificity	PPV	F1
CRP	0.5317	0.6879	0.2727	1	1	0.4286
PCT	0.5482	0.707	0.3939	0.9091	0.9286	0.5532
IL6	0.5895	0.7622	0.5455	0.7273	0.8571	0.6667
CRP+PCT+IL6	0.4904	0.6708	0.303	0.8182	0.8333	0.4444
Metabolite panel	0.7493	0.7211	0.8182	0.7273	0.9	0.8571
Metabolite panel+CRP	0.7355	0.6631	0.8182	0.7273	0.9	0.8571
Metabolite panel+PCT	0.741	0.7538	0.8182	0.8182	0.931	0.871
Metabolite panel+IL6	0.7851	0.6375	0.8485	0.8182	0.9333	0.8889

