

1 **Distinct global metabolomic profile of the model organism *Caenorhabditis elegans* during**  
2 **the interaction of *Staphylococcus aureus* and *Salmonella enteric* Serovar Typhi**  
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4 ***Krishnaswamy Balamurugan*<sup>1\*</sup>**

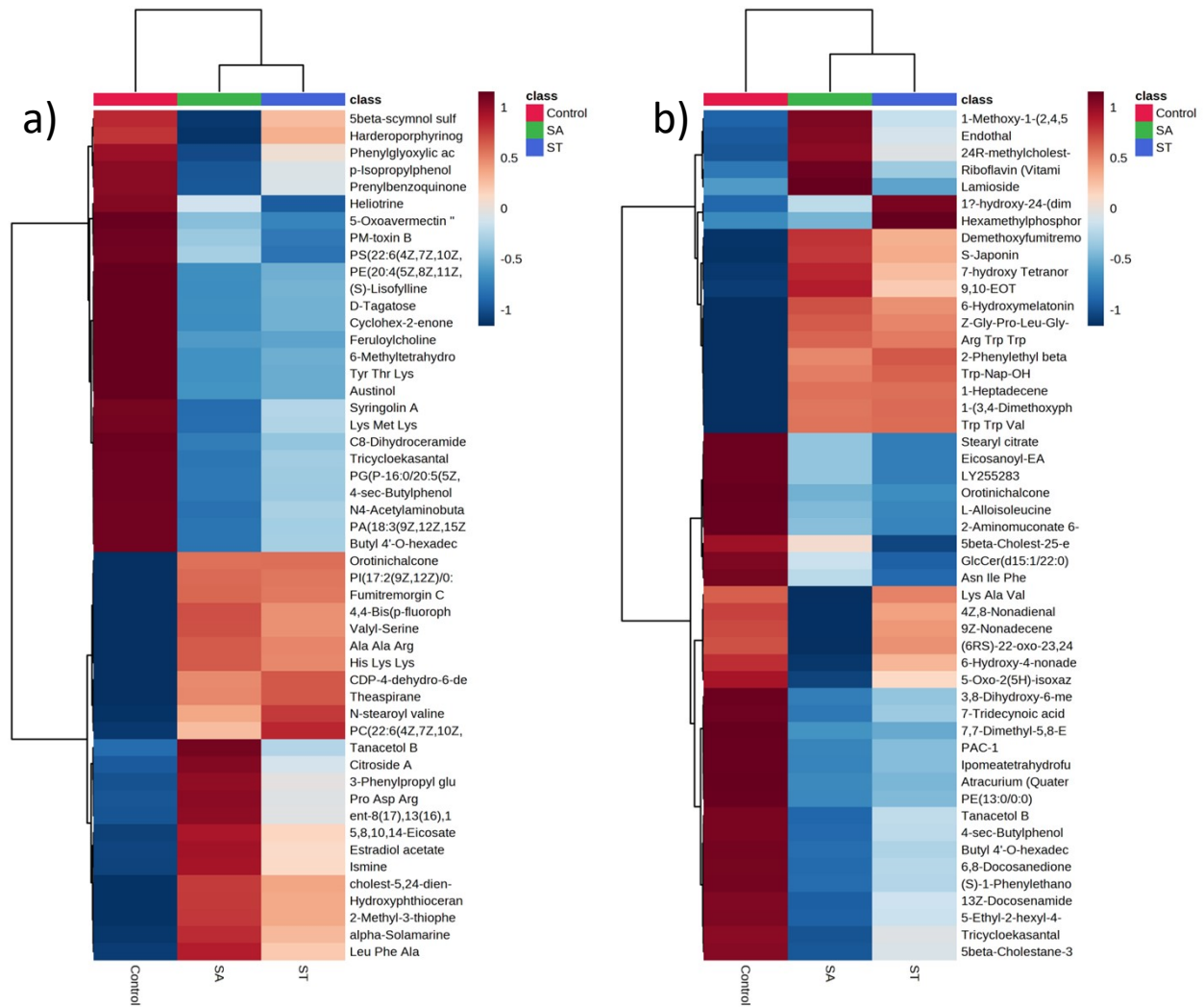
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8 **Supplementary files:**

9 **Supplementary Figure 1: Heatmap of significantly differ in expression pattern of top 50**  
10 **metabolites of a) endo-metabolome and b) exo-metabolome of *E. coli* OP50 exposed, *S.***  
11 ***aureus* exposed and *S. Typhi* exposed *C. elegans* (SA- *S. aureus*, ST- *S. Typhi*)**

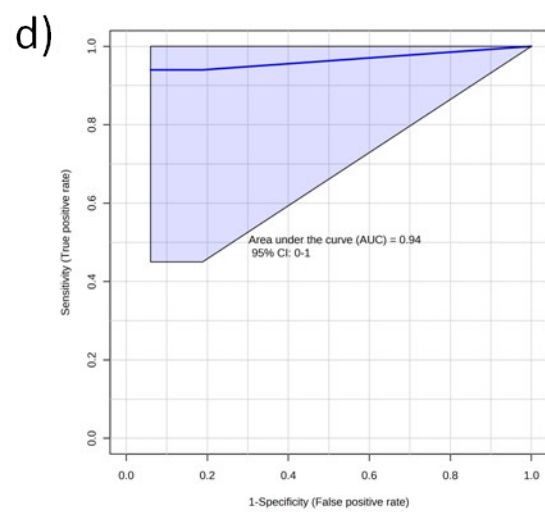
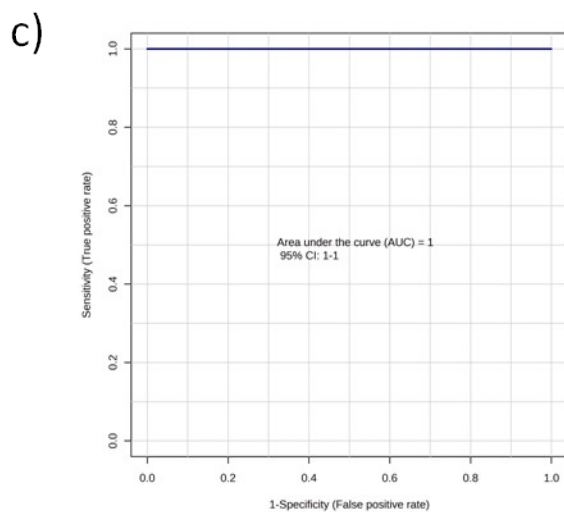
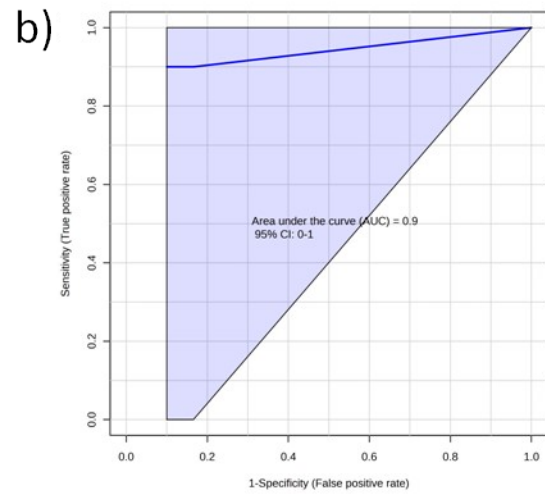
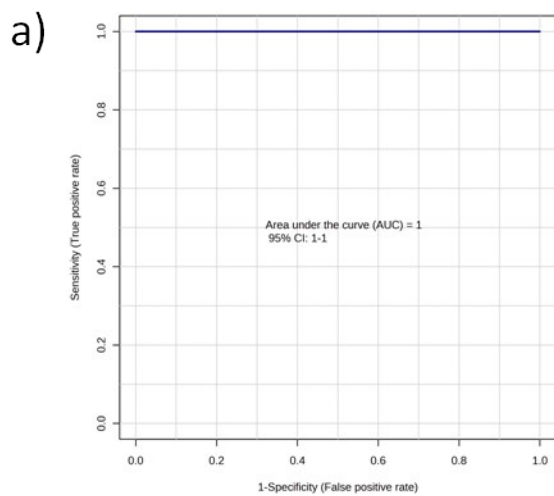


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15 **Supplementary Figure 2: Multivariate ROC analysis of 100 features (Cross validation**  
 16 **performance) with 95 % confident interval. ROC analysis of 100 features of endo-**  
 17 **metabolome of a) *S. aureus* & b) *S. Typhi* exposed *C. elegans*; exo-metabolome of c) *S.*  
 18 ***aureus* & d) *S. Typhi* exposed *C. elegans*.****



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21 **Supplementary table 1: Metabolites found exclusively in endo- and exo-metabolome of *E.***

22 ***coli* OP50 exposed, *S. aureus* exposed and *S. Typhi* exposed *C. elegans***

23 ***(A separate file has been attached)***

24 **Supplementary Table 2: Enriched metabolic pathways and most abundant identified**

25 **metabolites [endo- & exo- metabolome of *E. coli* OP50 exposed, *S. aureus* exposed and *S.***

26 ***Typhi* exposed *C. elegans***

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**Common Endo-metabolites of candidate pathogenic bacteria exposed *C. elegans* & *E. coli* OP50 fed *C. elegans***

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<b>Metabolism</b>	<b>Compounds identified</b>
Purine metabolism	Guanine, Guanosine, Adenosine diphosphate ribose, Adenine, 5-Aminoimidazole ribonucleotide, Deoxyadenosine
Arginine and proline metabolism	S-Adenosylmethioninamine, Spermidine, N4-Acetylaminobutanal, Pyrroline hydroxycarboxylic acid
Thiamine metabolism	Thiamine, Thiamine monophosphate
Sphingolipid metabolism	Sphingosine, 3-O-Sulfogalactosylceramide, Phytosphingosine
Drug metabolism - other enzymes	5-Fluorouridine, NPC, Isonicotinic acid
D-Arginine and D-ornithine metabolism	2-Oxoarginine
Phosphonate and phosphinate metabolism	Phosphocholine
Glycerophospholipid metabolism	Phosphorylcholine, Glycerophosphocholine
Caffeine metabolism	Paraxanthine
Tryptophan metabolism	Melatonin, 2-Aminomuconic acid semialdehyde
Histidine metabolism	N-Formyl-L-aspartate
Pentose and glucuronate interconversions	L-Threo-2-pentulose or L Xylulose
Selenocompound metabolism	Methylselenopyruvate
Ether lipid metabolism	Glycerophosphocholine
beta-Alanine metabolism	Spermidine
Lysine degradation	Saccharopine
Folate biosynthesis	Dihydroptericoic acid
Galactose metabolism	D-Tagatose 1,6-bisphosphate
Glutathione metabolism	Spermidine
Cysteine and methionine metabolism	S-Adenosylmethioninamine
N-Glycan biosynthesis	N-Acetyl-D-glucosaminyldiphosphodolichol
Tyrosine metabolism	Tyramine
Drug metabolism - cytochrome P450	p-Hydroxyfelbamate
Metabolism of xenobiotics by cytochrome P450	2-(S-Glutathionyl)acetyl chloride

Steroid hormone biosynthesis

2-Methoxyestrone 3-glucuronide

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**Common Exo-metabolites of candidate pathogenic bacteria exposed *C. elegans* and *E. coli* OP50 fed *C. elegans***

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Sphingolipid metabolism	Sphingosine, Phytosphingosine
D-Arginine and D-ornithine metabolism	2-Oxoarginine
Purine metabolism	Guanine, Adenine, Deoxyadenosine
Phosphonate and phosphinate metabolism	Phosphocholine
Glycerophospholipid metabolism	Phosphocholine, Glycerophosphocholine
Arginine and proline metabolism	N4-Acetylaminobutanal, Pyrroline hydroxycarboxylic acid
Drug metabolism - other enzymes	NPC, Isonicotinic acid
Tryptophan metabolism	2-Aminomuconic acid 6-semialdehyde, 6-Hydroxymelatonin
Histidine metabolism	N-Formyl-L-aspartate
Pentose and glucuronate interconversions	L-Threo-2-pentulose
Ether lipid metabolism	Glycerophosphocholine
Pentose phosphate pathway	6-Phosphonoglucono-D-lactone
Steroid hormone biosynthesis	Tetrahydrocortisone, 2-Methoxyestrone 3-glucuronide
N-Glycan biosynthesis	N-Acetyl-D-glucosaminyldiphosphodolichol
Drug metabolism - cytochrome P450	p-Hydroxyfelbamate

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**Exclusive in *E. coli* OP50 fed *C. elegans*' endo-metabolome and not in endo-metabolome candidate pathogenic bacteria exposed *C. elegans***

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Purine metabolism	2-(Formamido)-N1-(5-phospho-D-ribosyl)acetamidine, Deoxyinosine, Hypoxanthine, Inosine triphosphate, 2'-Deoxyinosine triphosphate, 5-hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate, Urea
Phenylalanine, tyrosine and tryptophan biosynthesis	Phenylpyruvic acid
Porphyrin and chlorophyll metabolism	Protoporphyrin IX, Coproporphyrinogen I
Drug metabolism - other enzymes	Irinotecan, alpha-Fluoro-beta-alanine
Vitamin B6 metabolism	2-Oxo-3-hydroxy-4-phosphobutanoic acid
Phenylalanine metabolism	Phenylpyruvic acid
Biotin metabolism	Biotin

Steroid hormone biosynthesis	21-Hydroxypregnenolone, Estrone sulfate, 2-Methoxyestrone 3-glucuronide
Arginine biosynthesis	Urea
Pentose and glucuronate interconversions	D-Xylitol
Terpenoid backbone biosynthesis	Farnesylcysteine
Galactose metabolism	Galactosylglycerol
Glycine, serine and threonine metabolism	Betaine aldehyde
N-Glycan biosynthesis	Dolichyl b-D-glucosyl phosphate
Tryptophan metabolism	5-Methoxyindoleacetate
Tyrosine metabolism	Epinephrine

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**Exclusive in *E. coli* OP50 exposed *C. elegans*' exo-metabolome and not in exo-metabolome of candidate pathogenic bacteria exposed *C. elegans***

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Pantothenate and CoA biosynthesis	Pantetheine 4'-phosphate, Pantothenic acid, D-4'-Phosphopantothenate, Uracil
Vitamin B6 metabolism	Pyridoxal 5'-phosphate, 2-Oxo-3-hydroxy-4-phosphobutanoic acid
Biotin metabolism	Biotin, Biocytin
Arginine biosynthesis	L-Glutamine, Urea
Purine metabolism	L-Glutamine, Deoxyinosine, Hypoxanthine, Urea
Phenylalanine, tyrosine and tryptophan biosynthesis	Phenylpyruvic acid
Steroid hormone biosynthesis	21-Hydroxypregnenolone, 5-Androstenediol, Estrone sulfate, 2-Methoxyestrone 3-glucuronide
D-Glutamine and D-glutamate metabolism	L-Glutamine
Nitrogen metabolism	L-Glutamine
Ubiquinone and other terpenoid-quinone biosynthesis	Vitamin K1
Pyrimidine metabolism	L-Glutamine, Uracil
N-Glycan biosynthesis	Dolichyl phosphate D-mannose, Dolichyl b-D-glucosyl phosphate
Drug metabolism - other enzymes	Irinotecan, alpha-Fluoro-beta-alanine
Caffeine metabolism	Caffeine
Phenylalanine metabolism	Phenylpyruvic acid

Glycosylphosphatidylinositol (GPI)-anchor biosynthesis	Dolichyl phosphate D-mannose
Mannose type O-glycan biosynthesis	Dolichyl phosphate D-mannose
Pentose and glucuronate interconversions	D-Xylitol
beta-Alanine metabolism	Uracil
Sphingolipid metabolism	Ceramide (d18:1/12:0)
Alanine, aspartate and glutamate metabolism	L-Glutamine
Glyoxylate and dicarboxylate metabolism	L-Glutamine
Fatty acid elongation	3-Oxotetradecanoyl-CoA
Arginine and proline metabolism	4-Hydroxyproline
Fatty acid degradation	3-Oxotetradecanoyl-CoA
Tryptophan metabolism	5-Hydroxy-L-tryptophan
Aminoacyl-tRNA biosynthesis	L-Glutamine
Drug metabolism - cytochrome P450	Citalopram aldehyde
Metabolism of xenobiotics by cytochrome P450	Aflatoxin B1exo-8,9-epoxide-GSH

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**Exclusive in *S. aureus* exposed *C. elegans* endo-metabolome not in endo-metabolome of *E. coli* OP50 & *S. Typhi* exposed *C. elegans***

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alpha-Linolenic acid metabolism	3-Oxo-OPC8-CoA, trans-2-Enoyl-OPC6-CoA
Ubiquinone and other terpenoid-quinone biosynthesis	Vitamin K1
One carbon pool by folate	Folic acid
Glycerolipid metabolism	TG(10:0/10:0/10:0)
Pentose and glucuronate interconversions	L-Arabinose
Selenocompound metabolism	Selenomethionine
Pyruvate metabolism	Acetylphosphate
Propanoate metabolism	Propinol adenylate
Folate biosynthesis	Folic acid
Porphyrin and chlorophyll metabolism	Cob(I)yrinate,c diamide
Pyrimidine metabolism	Thymine

Drug metabolism - cytochrome P450 2-Ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine

Steroid hormone biosynthesis Deoxycorticosterone

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**Exclusive in *S. aureus* exposed *C. elegans* exo-metabolome not in exo-metabolome of *E. coli* OP50 & *S. Typhi* exposed *C. elegans***

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Terpenoid backbone biosynthesis Dimethylallylpyrophosphate

beta-Alanine metabolism Spermidine

Glutathione metabolism Spermidine

Arginine and proline metabolism Spermidine

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**Exclusive in *S. Typhi* exposed *C. elegans* endo-metabolome not in endo-metabolome of *E. coli* OP50 & *S. aureus* exposed *C. elegans***

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Drug metabolism - cytochrome P450 4-Glutathionyl cyclophosphamide, Alcophosphamide, Citalopram propionic acid

Arginine and proline metabolism Phosphocreatine, 4-Guanidinobutanoic acid

Biotin metabolism Biocytin

alpha-Linolenic acid metabolism trans-2-Enoyl-OPC4-CoA

Arginine biosynthesis N-Acetylglutamic acid

Histidine metabolism 3-Methylhistidine

Terpenoid backbone biosynthesis Dimethylallylpyrophosphate

Pentose phosphate pathway 6-Phosphonoglucono-D-lactone

Phosphatidylinositol signaling system 1D-myo-Inositol 1,5-bis(diphosphate) 2,3,4,6-tetrakisphosphate

Porphyrin and chlorophyll metabolism Porphobilinogen

Fatty acid elongation Lauroyl-CoA

Fatty acid degradation Lauroyl-CoA

N-Glycan biosynthesis Dolichyl b-D-glucosyl phosphate

Tryptophan metabolism 6-Hydroxymelatonin

Purine metabolism Deoxyadenosine triphosphate

Steroid hormone biosynthesis Androsterone glucuronide

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**Exclusive in *S. Typhi* exposed *C. elegans* exo-metabolome not in exo-metabolome of *E. coli* OP50 & *S. aureus* exposed *C. elegans***

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Selenocompound metabolism Selenomethionine, Trimethylselenonium

Steroid hormone biosynthesis Tetrahydrocortisol, Androsterone glucuronide, Dehydroepiandrosterone



alpha-Linolenic acid metabolism	OPC4-CoA
Pantothenate and CoA biosynthesis	Pantetheine
Phosphatidylinositol signaling system	Phosphatidylinositol-3,4,5-trisphosphate
Inositol phosphate metabolism	Phosphatidylinositol-3,4,5-trisphosphate
Drug metabolism - other enzymes	5-Fluorouridine
Tryptophan metabolism	Melatonin
Tyrosine metabolism	Tyramine
Drug metabolism - cytochrome P450	4-Glutathionyl cyclophosphamide
Purine metabolism	5-Aminoimidazole ribonucleotide

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29 **Supplementary table 3: The significantly upregulated and downregulated metabolites of**  
30 **endo-metabolome during candidate pathogenic bacteria interaction than the control (*E.***  
31 ***coli* OP50 exposed *C. elegans*)**

Compound name (Up regulated in SA exposure)	Fold change (log 10)	Compound name (Down regulated in SA exposure)	Fold change (log 10)	Compound name (Up regulated in ST exposure)	Fold change (log 10)	Compound name (Down regulated in ST exposure)	Fold change (log 10)
						(S)-Lisofylline	-1.33066
						4-sec-Butylphenol	-1.5261
2-Methyl-3- thiophenethiol	0.584736	(S)-Lisofylline	-1.71503	2-Methyl-3-thiophenethiol	0.463019	5beta-scymanol sulfate	-0.35263
3-Phenylpropyl glucosinolate	0.690747	4-sec-Butylphenol	-3.50211	3-Phenylpropyl glucosinolate	0.036654	5-Oxoavermectin "1b" aglycone	-0.14162
4,4-Bis(p- fluorophenyl)butyric acid	0.291838	5beta-scymanol sulfate	-2.16221	4,4-Bis(p- fluorophenyl)butyric acid	0.208235	6- Methyltetrahydropterin	-1.20552
5,8,10,14- Eicosatetraenoic acid, 12-hydroxy-, (E,Z,Z,Z)-; 12-HETE; 12-Hydroxy- 5,8,10,14- eicosatetraenoic acid; 12- Hydroxyeicosatetraenoic acid	0.911476	5-Oxoavermectin "1b" aglycone	-0.93058	5,8,10,14-Eicosatetraenoic acid, 12-hydroxy-, (E,Z,Z,Z)-; 12-HETE; 12-Hydroxy- 5,8,10,14-eicosatetraenoic acid; 12- Hydroxyeicosatetraenoic acid	0.325073	Austinol	-1.43394
Ala Ala Arg	0.332969	6- Methyltetrahydropterin	-1.29108	Ala Ala Arg	0.294183	Butyl 4'-O- hexadecanoyl- neohesperidoside	-1.08807
alpha-Solamarine	0.430817	Austinol	-1.6803	alpha-Solamarine	0.27594	C8-Dihydroceramide	-1.60567
CDP-4-dehydro-6-deoxy- D-glucose	0.295421	Butyl 4'-O- hexadecanoyl- neohesperidoside	-2.59356	CDP-4-dehydro-6-deoxy-D- glucose	0.445594	Cyclohex-2-enone	-1.14363

cholest-5,24-dien-3beta-ol 3-O-beta-D-glucopyranoside	0.43896	C8-Dihydroceramide	-2.11284	cholest-5,24-dien-3beta-ol 3-O-beta-D-glucopyranoside	0.344063	D-Tagatose	-1.5429
Citroside A	0.847243	Cyclohex-2-enone	-1.20331	Citroside A	0.052325	Feruloylcholine	-1.14838
ent-8(17),13(16),14-Labdatrien-18-oic acid	1.119253	D-Tagatose	-2.10021	ent-8(17),13(16),14-Labdatrien-18-oic acid	0.256008	Harderoporphyrinogen	-0.28927
Estradiol acetate	0.492893	Feruloylcholine	-1.32584	Estradiol acetate	0.040643	Heliotrine	-1.5321
Fumitremorgin C	0.243259	Harderoporphyrinogen	-2.27447	Fumitremorgin C	0.335692	Lys Met Lys	-1.37724
His Lys Lys	0.426283	Heliotrine	-0.90589	His Lys Lys	0.316375	N4-Acetylaminobutanal	-1.31069
Hydroxyphthioceranic acid (C39)	0.890869	Lys Met Lys	-2.03929	Hydroxyphthioceranic acid (C39)	0.637303	PA(18:3(9Z,12Z,15Z)/17:2(9Z,12Z))	-1.26358
Ismine	0.455505	N4-Acetylaminobutanal	-1.93232	Ismine	0.057552	PG(P-16:0/20:5(5Z,8Z,11Z,14Z,17Z))	-1.10612
Leu Phe Ala	0.696486	PA(18:3(9Z,12Z,15Z)/17:2(9Z,12Z))	-1.62984	Leu Phe Ala	0.318072	Phenylglyoxylic acid	-0.57203
N-stearoyl valine	0.024244	PG(P-16:0/20:5(5Z,8Z,11Z,14Z,17Z))	-2.01468	N-stearoyl valine	0.247816	p-Isopropylphenol	-0.67252
Orotinichalcone	0.977633	Phenylglyoxylic acid	-1.78879	Orotinichalcone	1.02651	PM-toxin B	-1.28172
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/13:0)	0.192519	p-Isopropylphenol	-4.29213	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/13:0)	0.585626	Prenylbenzoquinone	-0.52132
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0)	0.049322	PM-toxin B	-1.11612	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0)	0.63848	PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	-1.44835
PI(17:2(9Z,12Z)/0:0)	0.315335	Prenylbenzoquinone	-3.17291	PI(17:2(9Z,12Z)/0:0)	0.333648	Syringolin A	-1.05657
Pro Asp Arg	0.351919	PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	-1.03664	Theaspirane	0.958223	Tricycloekasantal	-1.7397
Tanacetol B	0.456605	Syringolin A	-2.08308	Valyl-Serine	0.449849	Tyr Thr Lys	-1.4578
Theaspirane	0.678695	Tricycloekasantal	-2.88689			Pro Asp Arg	-0.13271
Valyl-Serine	0.564426	Tyr Thr Lys	-1.64205			Tanacetol B	-0.25358

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33 **Supplementary table 4: The significantly upregulated and downregulated metabolites of**  
34 **exo-metabolome during candidate pathogenic bacteria interaction than the control (*E. coli***  
35 **OP50 exposed *C. elegans*).**

Compound name (Up regulated in SA exposure)	Fold change (log 10)	Compound name (Down regulated in SA exposure)	Fold change (log 10)	Compound name (Down regulated in ST exposure)	Fold change (log 10)	Compound name (Up regulated in ST infected)	Fold change (log 10)
1-(3,4-Dimethoxyphenyl)-1,2-ethanediol 1-O-b-D-glucoside	0.428786	(6RS)-22-oxo-23,24,25,26,27-pentanorvitamin D3 6,19-sulfur dioxide adduct / (6RS)-22-oxo-23,24,25,26,27-pentanorcholecalciferol 6,19-sulfurdioxide adduct	-1.93672	(6RS)-22-oxo-23,24,25,26,27-pentanorvitamin D3 6,19-sulfur dioxide adduct / (6RS)-22-oxo-23,24,25,26,27-pentanorcholecalciferol 6,19-sulfurdioxide adduct	-0.08874	1-(3,4-Dimethoxyphenyl)-1,2-ethanediol 1-O-b-D-glucoside	0.351605
1-Heptadecene	0.452724	(S)-1-Phenylethanol	-2.22319	(S)-1-Phenylethanol	-0.472	1-Heptadecene	0.330151
1-Methoxy-1-(2,4,5-trimethoxyphenyl)-2-propanol	0.965471	13Z-Docosenamide	-2.62022	13Z-Docosenamide	-1.27589	1-Methoxy-1-(2,4,5-trimethoxyphenyl)-2-propanol	0.042796
24R-methylcholest-22E-en-3beta,4beta,5alpha,6alpha,8beta,14alpha,15alpha,25R	0.928296	1α-hydroxy-24-(dimethoxyphosphoryl)-25,26,27-trinorvitamin D3 / 1α-hydroxy-24-	-0.11133	2-Aminomuconate 6-semialdehyde	-1.26691	Hexamethylphosphoramide	1.066289

,26-nonol		(dimethoxyphosphoryl)-25,26,27-trinorcholecalciferol				
2-Phenylethyl beta-D-glucopyranoside	0.257579	2-Aminomuconate 6-semialdehyde	-0.95941	3,8-Dihydroxy-6-methoxy-7(11)-eremophilen-12,8-olide	-1.33323	2-Phenylethyl beta-D-glucopyranoside 0.328514
6-Hydroxymelatonin	0.283146	3,8-Dihydroxy-6-methoxy-7(11)-eremophilen-12,8-olide	-1.48411	4-sec-Butylphenol	-0.63387	6-Hydroxymelatonin 0.160474
7-hydroxy Tetranorlloprost	0.709466	4-sec-Butylphenol	-2.69327	4Z,8-Nonadienal	-0.2823	7-hydroxy Tetranorlloprost 0.267326
9,10-EOT	0.930467	4Z,8-Nonadienal	-1.06848	5beta-Cholest-25-ene-3alpha,7alpha,12alpha,26-tetrol	-1.65311	9,10-EOT 0.326302
Arg TrpTrp	0.22936	5beta-Cholest-25-ene-3alpha,7alpha,12alpha,26-tetrol	-0.4481	5beta-Cholestane-3alpha,26-diol	-0.86506	Arg TrpTrp 0.15541
Demethoxyfunitremorgin C	0.523887	5beta-Cholestane-3alpha,26-diol	-1.46482	5-Ethyl-2-hexyl-4-methyloxazole	-0.32983	Demethoxyfunitremorgin C 0.199925
Lamioside	0.476462	5-Ethyl-2-hexyl-4-methyloxazole	-3.75027	5-Oxo-2(5H)-isoxazolepropanenitrile	-0.46799	1alpha-hydroxy-24-(dimethoxyphosphoryl)-25,26,27-trinorvitamin D3 / 1alpha-hydroxy-24-(dimethoxyphosphoryl)-25,26,27-trinorcholecalciferol 0.591177
Riboflavin (Vitamin B2)	0.601615	5-Oxo-2(5H)-isoxazolepropanenitrile	-1.13671	6,8-Docosanedione	-1.15321	S-Japonin 0.394269
S-Japonin	1.054933	6,8-Docosanedione	-2.29053	6-Hydroxy-4-nonadecanone	-0.26873	TrpTrp Val 0.230647
TrpTrp Val	0.280488	6-Hydroxy-4-nonadecanone	-1.74213	7,7-Dimethyl-5,8-Eicosadienoic Acid	-1.11901	Trp-Nap-OH 0.228575
Trp-Nap-OH	0.236097	7,7-Dimethyl-5,8-Eicosadienoic Acid	-1.50148	7-Tridecynoic acid	-1.3257	Z-Gly-Pro-Leu-Gly-Pro 0.010976
Z-Gly-Pro-Leu-Gly-Pro	0.135713	7-Tridecynoic acid	-1.334	9Z-Nonadecene	-0.06466	
		9Z-Nonadecene	-1.92597	Asn Ile Phe	-2.39073	
		Asn Ile Phe	-1.58698	Atracurium (Quaternary acid)	-1.78443	
		Atracurium (Quaternary acid)	-1.92172	Butyl 4'-O-hexadecanoyl-neohesperidoside	-1.15873	
		Butyl 4'-O-hexadecanoyl-neohesperidoside	-2.74982	Eicosanoyl-EA	-2.54928	
		Eicosanoyl-EA	-1.98939	GlcCer(d15:1/22:0)	-2.44808	
		GlcCer(d15:1/22:0)	-1.04321	Ipomeatetrahydrofuran	-1.20838	
		Hexamethylphosphoramidate	-0.1967	L-Alloisoleucine	-1.34798	
		Ipomeatetrahydrofuran	-1.77517	LY255283	-1.28955	
		L-Alloisoleucine	-1.24423	Lys Ala Val	-0.03017	
		LY255283	-1.06476	Orotinichalcone	-2.23979	
		Lys Ala Val	-1.75849	PAC-1	-2.04836	
		Orotinichalcone	-1.89731	PE(13:0/0:0)	-2.30978	
		PAC-1	-2.22259	Stearyl citrate	-1.53054	
		PE(13:0/0:0)	-2.76055	Tanacetol B	-0.8456	
		Stearyl citrate	-0.69271	Tricycloekasantal	-0.23168	
		Tanacetol B	-1.17684	Lamioside	-0.42487	
		Tricycloekasantal	-3.46125	Riboflavin (Vitamin B2)	-0.18396	
				24R-methylcholest-22E-en-3beta,4beta,5alpha,6alpha,8beta,14alpha,15alpha,25R,26-nonol	-0.0027	

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