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SUPPLEMENTARY MATERIAL

Identification of Bioactive Postbiotics Against Neonatal Meningitis Caused by Group B *Streptococcus via* Srr2-Targeted *In silico* Screening

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Table S1. Physiochemical properties of target protein *Srr2*.

Serine-rich repeat protein (*Srr2*)	
Number of Amino acids	344
Molecular Weight	38442.52
Theoretical PI	4.8
Extinction Coefficient (assuming all Cys residues form Cystines)	46300
Extinction Coefficient (assuming all Cys residues are reduced)	45930
Instability Index	25.64
Aliphatic Index	78.14
Grand Average of Hydropathicity (GRAVY)	-0.522
Total number of negatively charged residues (Asp + Glu)	49
Total number of Positively charged residues (Arg + Lys)	30

Table S2. CB Dock 2 with ligands name, binding score, and cavity size.

Sr. No.	Ligands name	Binding score	Cavity size
1	Citric acid	-7.3	6126
2	Arachidonic acid	-6.3	6126
3	Palmitoleic acid	-5.8	354
4	Palmitic acid	-5.5	6126
5	Lauric acid	-5.4	6126
6	Linoleic acid	-5.4	6126
7	Oleic acid	-5.2	6126
8	Malic acid	-5	6126

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Table S3A. Absorption properties comparison.

Properties	Cefotaxime	Citric Acid
Water solubility	-2.576	-1.423
$CaCO_2$ permeability	-0.461	-0.24
Intestinal absorption	37.939	90.21
Skin permeability	-2.735	-2.735
p-glycoprotein substrate	Yes	No
p-glycoprotein I inhibitor	No	No
p-glycoprotein II inhibitor	No	No

Table S3B. Distribution properties comparison.

Properties	Cefotaxime	Citric Acid
VDss (human)	-1.744	0.418
Fraction unbound (human)	0.563	0.104
BBB permeability	-1.713	-1.017
CNS permeability	-3.967	-3.61

Table S3C. Metabolic properties comparison.

Properties	Cefotaxime	Citric Acid
CYP2D6 substrate	No	No
CYP3A4 substrate	No	No
CYP1A2 inhibitor	No	No
CYP2C19 inhibitor	No	No
CYP2C9 inhibitor	No	No
CYP3A4 inhibitor	No	No

Table S3D. Excretion properties comparison.

Properties	Cefotaxime	Citric Acid
Total clearance	0.015	0.895
Renal OCT2 substrate	No	No

Table S3E. Toxicity properties comparison.

Properties	Cefotaxime	Citric Acid
AMES toxicity	No	No
Max. tolerated dose (human)	1.608	0.749
HERG I Inhibitor	No	No
HERG II inhibitor	No	No
Oral rat acute toxicity (LD50)	1.933	2.148
Oral rat Chronic toxicity (LOAEL)	2.359	3.698
Hepatotoxicity	Yes	No
Skin sensitization	No	No
T. *pyriformis* toxicity	0.285	0.285
Minnow toxicity	4.653	4.251