

Supplementary Materials

Inhibition of Cellular Proliferation by No. 4	
IC ₅₀ [μM]	
HL60	HEK293
64.9	161.3

Supplementary Table ST1. Cellular effect of compound no. 4. MTT test demonstrating the anti-leukemic effects of Conjugate 4 compared to its impact on non-cancerous embryo cells after 72 hours of incubation; The initial cellular density for HL60 was 5,000 cells, and for HEK293, it was 1,500 cells per well, respectively; IC₅₀ - Inhibitory Concentration; Values represent averages ±SEM from five independent biological experiments in technical triplicate; n/d - not determined.

Effective Concentration IC ₅₀ [nM]				
No.	HL60	BT20	A549	HEK293
LfcinB	10	77	151	499
1	8	24	69	307
2	8	22	257	322
3	3	22	37	409
4	13	40	50	108

Supplementary Table ST2. Effective concentration values. The conversion from IC₅₀ to EC₅₀ was performed following the method outlined in [62]; For IC₅₀ values, please refer to Supplementary Table ST1 and the corresponding reference [61]; IC₅₀ - Inhibitory Concentration; EC₅₀ - Effective Concentration.

Antimicrobial Selectivity Index												
No.	Bacteriostatic Normalized to IC ₅₀						Fungistatic Normalized to IC ₅₀					
	HL60											
	S. e.	B. s.	S. a.	E. c.	P. a.	B. c.	C. k.	C. p.	C. a.	C. g.	C. t.	
LfcinB	11.5	0.7	0.7	2.9	2.9	0.7	0.7	0.7	0.7	0.7	0.7	
1	5.7	0.7	0.7	0.7	0.7	0.7	2.9	1.4	0.7	0.7	0.7	
2	12.9	3.2	3.2	0.8	0.8	0.8	1.6	0.8	0.8	0.8	0.8	
3	11.6	1.5	1.5	1.5	0.7	0.4	0.7	0.4	0.4	0.4	0.4	
4	9.5	2.4	1.2	4.8	4.8	1.2	2.4	1.2	1.2	1.2	1.2	
	BT20											
LfcinB	27.5	1.7	1.7	6.9	6.9	1.7	1.7	1.7	1.7	1.7	1.7	
1	5.2	0.7	0.7	0.7	0.7	0.7	2.6	1.3	0.7	0.7	0.7	
2	10.3	2.5	2.5	0.6	0.6	0.6	1.3	0.6	0.6	0.6	0.6	
3	25.1	3.2	3.2	3.2	1.6	0.8	1.6	0.8	0.8	0.8	0.8	
4	8.8	2.2	1.1	4.4	4.4	1.1	2.2	1.1	1.1	1.1	1.1	
	A549											
LfcinB	53.9	3.4	3.4	13.6	13.6	3.4	3.4	3.4	3.4	3.4	3.4	
1	15.3	1.9	1.9	1.9	1.9	1.9	7.7	3.8	1.9	1.9	1.9	
2	120.6	29.7	29.7	7.5	7.5	7.5	14.9	7.5	7.5	7.5	7.5	
3	43.2	5.5	5.5	5.5	2.8	1.4	2.8	1.4	1.4	1.4	1.4	
4	11.0	2.8	1.4	5.5	5.5	1.4	2.8	1.4	1.4	1.4	1.4	
	HEK293											
LfcinB	178.1	11.2	11.2	44.8	44.8	11.2	11.2	11.2	11.2	11.2	11.2	
1	67.8	8.5	8.5	8.5	8.5	8.5	33.9	17.0	8.5	8.5	8.5	
2	150.8	37.1	37.1	9.3	9.3	9.3	18.6	9.3	9.3	9.3	9.3	
3	471.5	60.1	60.1	60.1	30.0	15.0	30.0	15.0	15.0	15.0	15.0	
4	23.7	6.0	3.0	11.9	11.9	3.0	6.0	3.0	3.0	3.0	3.0	

Citation: To be added by editorial staff during production.

Academic Editor: Firstname Last-name

Received: date

Revised: date

Accepted: date

Published: date



Copyright: © 2023 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

Supplementary Table ST3. Antimicrobial Selectivity Index of LfcinB and selected conjugates in relation to IC₅₀ values for HL60, BT20, A549, and HEK293. For MIC and IC₅₀ data, please also refer to Ptaszynska et al., 2019. Abbreviations: S. e. - *Staphylococcus epidermidis* ATCC 12228; B. s. - *Bacillus subtilis* ATCC 6633; S. a. - *Staphylococcus aureus* ATCC 25923; P. a. - *Pseudomonas aeruginosa* ATCC 27853; B. c. - *Bacillus cereus* PCM 2003; C. k. - *Candida krusei* DSM 6128; C. p. - *Candida parapsilosis* DSM 5784; C. a. - *Candida albicans* ATCC 10231; C. g. - *Candida glabrata* DSM 11226; C. t. - *Candida tropicalis* CZD 519.

Malignancy Selectivity Index				
No.	HL60			
	HL-60	BT20	A549	HEK293
LfcinB	n/d	8.0	15.6	51.6
1	n/d	3.0	8.9	39.4
2	n/d	2.7	31.1	38.8
3	n/d	7.2	12.4	135.3
4	n/d	3.1	3.8	8.3
BT20				
	HL-60	BT20	A549	HEK293
LfcinB	0.1	n/d	2.0	6.5
1	0.3	n/d	2.9	13.1
2	0.4	n/d	11.7	14.6
3	0.1	n/d	1.7	18.8
4	0.3	n/d	1.2	2.7
A549				
	HL-60	BT20	A549	HEK293
LfcinB	0.1	0.5	n/d	3.3
1	0.1	0.3	n/d	4.4
2	0.0	0.1	n/d	1.3
3	0.1	0.6	n/d	10.9
4	0.3	0.8	n/d	2.2
HEK293				
	HL-60	BT20	A549	HEK293
LfcinB	0.0	0.2	0.3	n/d
1	0.0	0.1	0.2	n/d
2	0.0	0.1	0.8	n/d
3	0.0	0.1	0.1	n/d
4	0.1	0.4	0.5	n/d

Supplementary Table ST4. Normalized to EC₅₀ Malignancy Selectivity Index.

Compound	MW [g/mol] (found/calc.)	t _R [min]	Yield %
CIP	331.4	11.3	--
LVX	361.4	11.2	--
FLC	306.3	10.7	--
FLC-COOH	365.2/364	11.8	46%
CIP-Cys	435.3/434.5	29.3	92%
LfcinB(2-11)-NH ₂	1496.9/1495.8	14.3	90-95%
Nle- LfcinB-NH ₂	2017.8/2017.5	15.3	
1	1841.2/1839.2	15.6	4%
2	1929.6/1929.8	16.2	30%
3	2452.2/2451.5	15.5	30%
4	1843.6/1841.8	18.3	73%

Supplementary Table ST5. Physicochemical properties of peptide conjugates and its components.

Supplementary Figure S1. MS analysis of peptide and peptide conjugates and their constituents. (a) CIP-Cys; (b) LfcinB(2-11)-NH₂; (c) Nle- LFcInB-NH₂; (d) 1; (e) 2; (f) 3; (g) 4.







