

## **Supplementary materials**

### **De novo design of AC-P19M, a novel anticancer peptide, with apoptotic effect on lung cancer cells and anti-angiogenic activity**

**Table S1. Six template sequences aligned from 15-mer to 20-mer anticancer peptides**

**Table S2. Representative results of functional prediction by machine learning-based web tools**

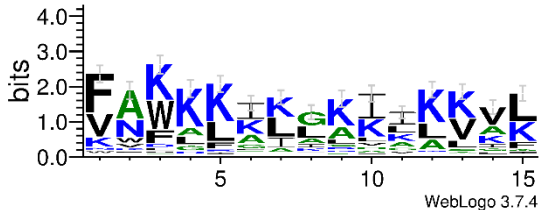
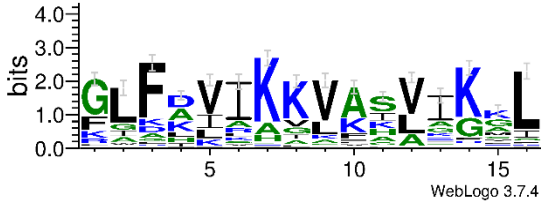
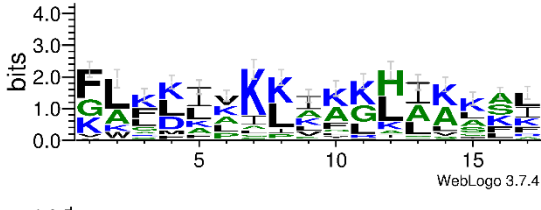
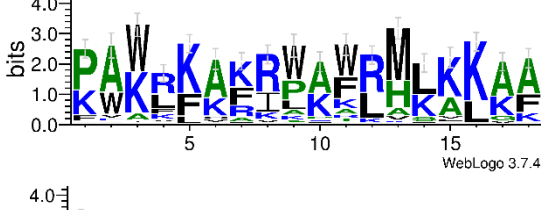
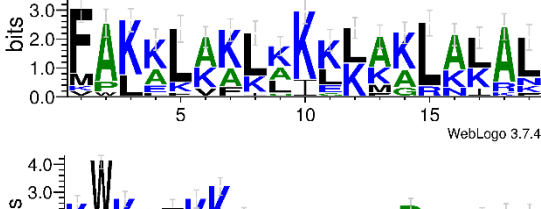
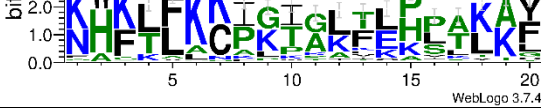
**Table S3. Minimum inhibitory concentration and minimum bactericidal concentration of AC-P19 and AC-P19M**

**Figure S1. Three-dimensional modeling of AC-P19 and AC-P19M**

**Figure S2. Cell cycle assay of A549 and H460 upon AC-P19M treatment**

**Figure S3. Field emission-scanning electron imaging of bacteria upon AC-P19M treatment**

Table S1. Six template sequences aligned from 15-mer to 20-mer anticancer peptides

Peptide	Aligned sequence	
15-mer	FAKKIKGKIIKKVL	 WebLogo 3.7.4
16-mer	GLFDVIKKVASVIKKL	 WebLogo 3.7.4
17-mer	FLKKIVKKIKKHIKKAL	 WebLogo 3.7.4
18-mer	PAWRKAKRWAWRMLKAA	 WebLogo 3.7.4
19-mer (AC-P19)	FAKKLAKLKKKLAKLALAL	 WebLogo 3.7.4
20-mer	KWKLFKKIGIGLTLPPAKAY	 WebLogo 3.7.4

**Table S2. Representative results of functional prediction by machine learning-based web tools**

Length (AA)	Sequence	Anticancer activity			Cell penetrating activity			Hemolysis		
		mACPpred	ACPred	ENNACT	CellPPD	BChemRF- CPPred	MLCPP	HAPPENN	DBAASP (erythrocyte)	HemoPI
15	<u>FAKKIKGKIIKKVL*</u>	0.9768	1	1.000	0.05 (CPP)	87.05%	0.8758	0.012	0.76 (PPV)	0.47
	FAKKIKGKIIKKVR	0.9603	1	1.0	0.05 (CPP)	89.3%	0.9082	0.006	0.85 (PPV)	0.48
	FAKKIKGKIIKKVLR	0.9796	1	1.0	0.05 (CPP)	89.37%	0.9186	0.012	0.85 (PPV)	0.47
16	<u>GLFDVIKKVASVIKKL</u>	0.9827	1	1.000	0.05 (CPP)	70.16%	0.4522	0.490	0.62 (NPV)	0.64
	GLFDVIKKVASVIKKR	0.9825	0.999	0.999	0.05 (CPP)	66.09%	0.5424	0.115	0.77 (PPV)	0.58
	GLFDVIKKVASVIKKLR	0.9797	0.998	1.0	0.05 (CPP)	62.62%	0.5225	0.302	0.50 (PPV)	0.56
17	<u>FLKKIVKKIKKHIKKAL</u>	0.9781	1	1.000	0.05 (CPP)	53.82%	0.9167	0.176	0.71 (PPV)	0.47
	FLKKIVKKIKKHIKKAR	0.9812	1	1.0	0.05 (CPP)	55.76%	0.9412	0.103	0.82 (PPV)	0.47
	FLKKIVKKIKKHIKKALR	0.9801	1	1.0	0.05 (CPP)	57.08%	0.9416	0.183	0.73 (PPV)	0.45
18	<u>PAWRKAKRWAWRMLKKA</u>	0.9786	0.973	1.000	0.05 (CPP)	92.01%	0.9634	0.014	0.83 (PPV)	0.49
	PAWRKAKRWAWRMLKKAR	0.9787	0.912	1.0	0.05 (CPP)	93.61%	0.9795	0.008	0.96 (PPV)	0.49
	PAWRKAKRWAWRMLKKAAR	0.9795	0.961	1.0	0.05 (CPP)	93.3%	0.9757	0.008	0.88 (PPV)	0.49
19	<u>FAKKLAKLKKKLAKLALAL**</u>	0.9813	0.992	1.000	0.05 (CPP)	88.47%	0.9797	0.020	0.55 (NPV)	0.62
	FAKKLAKLKKKLAKLALAR	0.9829	0.986	1.0	0.05 (CPP)	90.6%	0.9752	0.009	0.70 (PPV)	0.62
	FAKKLAKLAKKLAKLAKR***	0.9806	0.999	1.0	0.05 (CPP)	92.32%	0.9808	0.008	0.84 (PPV)	0.57

20	<u>KWKLFKKIGIGLTLPPAKAY</u>	0.9786	0.986	0.159	0.05 (CPP)	68.97%	0.6384	0.004	0.68 (PPV)	0.48
	KWKLFKKIGIGLTLPPAKAR	0.9781	0.908	0.251	0.05 (CPP)	63.91%	0.7379	0.002	0.85 (PPV)	0.47
	KWKLFKKIGIGLTLPPAKAYR	0.9795	0.969	0.362	0.05 (CPP)	64.03%	0.7292	0.003	0.68 (PPV)	0.50

\* Underlined sequences represent aligned template sequences

\*\* AC-P19

\*\*\* AC-P19M

**Table S3. Minimum inhibitory concentration and minimum bactericidal concentration of AC-P19 and AC-P19M**

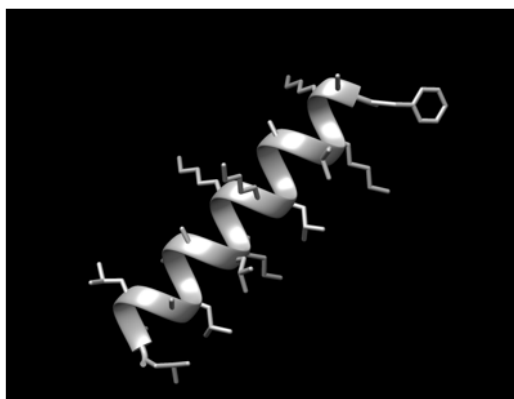
<b>Peptide</b>	<i>Escherichia coli</i>		<i>Pseudomonas aeruginosa</i>		<i>Bacillus subtilis</i>	
	MIC*	MBC**	MIC	MBC	MIC	MBC
AC-P19	1	2	4	8	2	2
AC-P19M	4	32	1	2	1	1

\* Minimum inhibitory concentration (μM)

\*\* Minimum bactericidal concentration (μM)

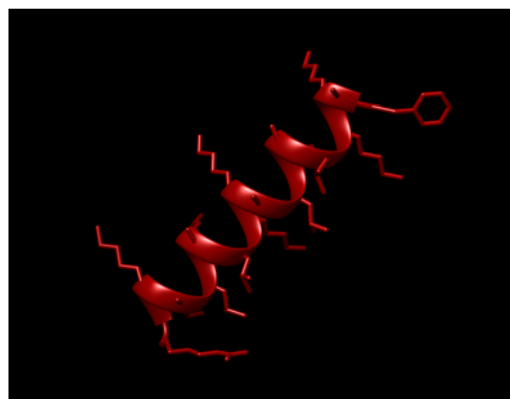
Figure S1. Three-dimensional modeling of AC-P19 and AC-P19M

**A**



AC-P19

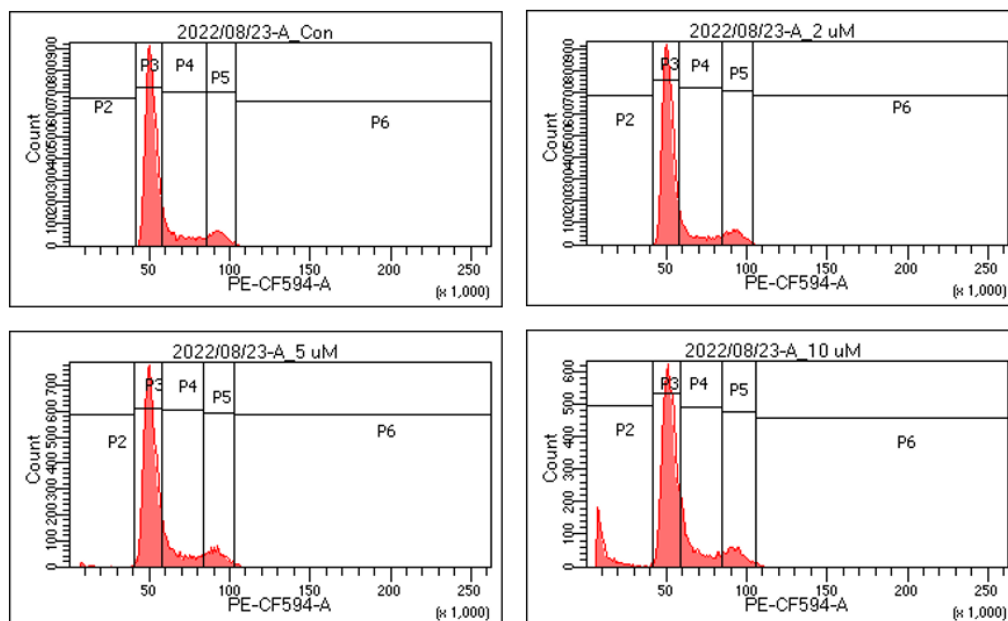
**B**



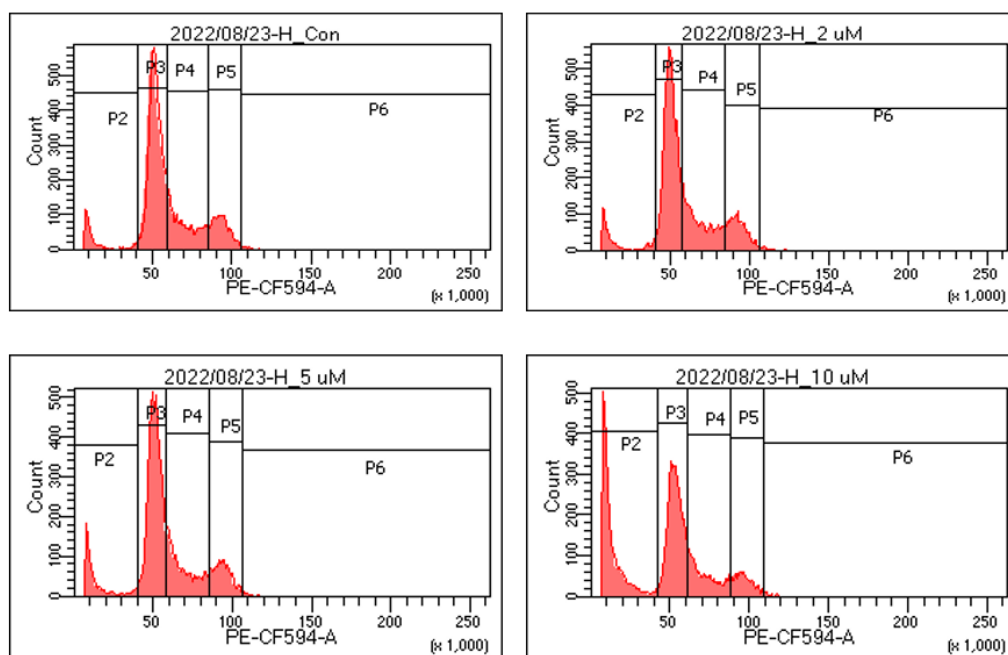
AC-P19M

Figure S2. Cell cycle assay of A549 and H460 upon AC-P19M treatment

**A**



**B**



**Figure S3. Field emission-scanning electron imaging of bacteria upon AC-P19M treatment**

