

**Table S1** Experimental table of response surface methodology

Factors	levels		
	-1	0	1
CPP/Calcium (mg/mg CPP)	1:2	1:4	1:6
pH	7.5	8	8.5
Temperature (°C)	20	30	40
Time (min)	10	20	30

**Table S2** Results of regression and variance analysis

	Sum of squares	Variance	Mean square	F value	Pr>F	Significant
Model	0.3485	14	0.0249	6.9113	0.0004	Significant
A	0.2187	1	0.2187	60.7228	< 0.0001	**
B	0.0044	1	0.0044	1.2210	0.2878	
C	0.0286	1	0.0286	7.9309	0.0137	*
D	0.0083	1	0.0083	2.3053	0.1512	
AB	0.0001	1	0.0001	0.0411	0.8423	
AC	0.0122	1	0.0122	3.3796	0.0873	
AD	0.0237	1	0.0237	6.5712	0.0225	*
BC	0.0007	1	0.0007	0.1869	0.6721	
BD	0.0006	1	0.0006	0.1691	0.6871	
CD	0.0170	1	0.0170	4.7255	0.0474	*
A <sup>2</sup>	0.0174	1	0.0174	4.8190	0.0455	*
B <sup>2</sup>	0.0030	1	0.0030	0.8304	0.3776	
C <sup>2</sup>	0.0038	1	0.0038	1.0607	0.3205	
D <sup>2</sup>	0.0039	1	0.0039	1.0698	0.3185	
Residue	0.0504	14	0.0036			
Lack of fit	0.0449	10	0.0045	3.2588	0.1331	Not significant
Pure error	0.0055	4	0.0014			
Core total	0.3990	28				

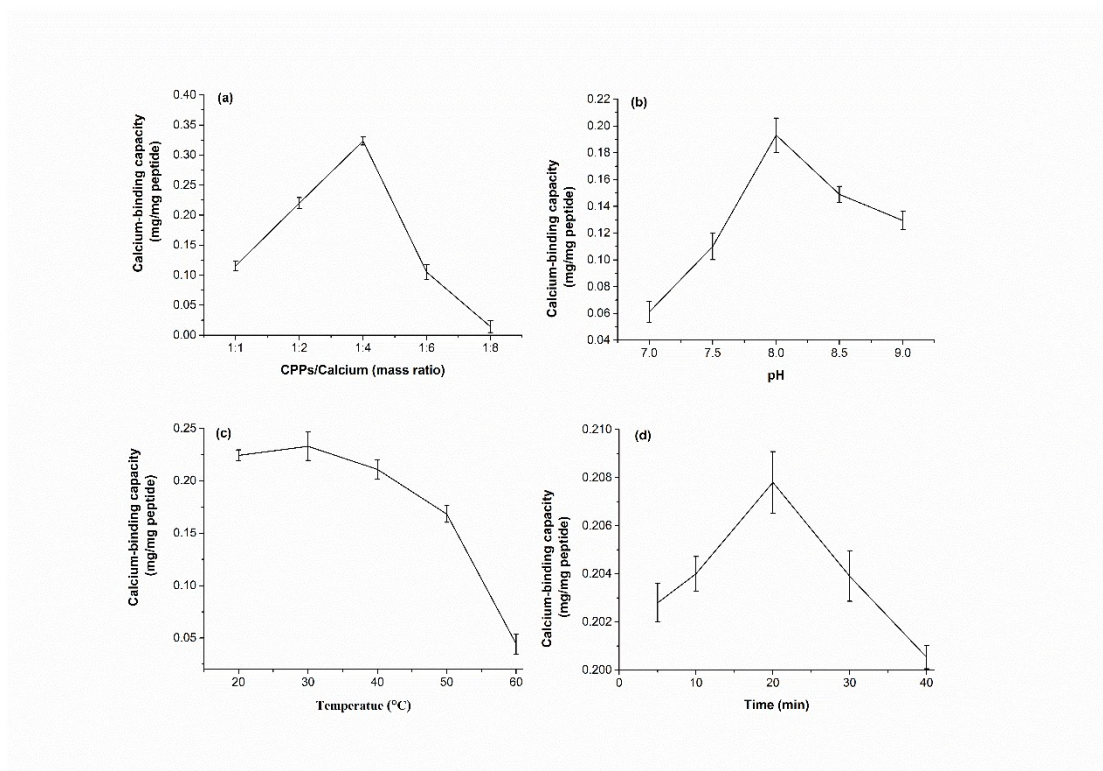
P<0.01: \*\* extremely significant; P<0.05: \* significant; P>0.05: Not significant.

## Figure captions

**Figure S1** Effects of the mass ratios of (a) CPPs/calcium, (b) pH, (c) temperature and (d) time on calcium-binding capacity of CPPs

**Figure S2** The four representative snapshots selected among 5000 structures from five trajectories evaluated by SPICKER software.

**Figure S1**



**Figure S2**

