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**Electronic Supplementary Information**

**Dual functional peptide carrying *in vitro* selected catalytic  
and binding activities**

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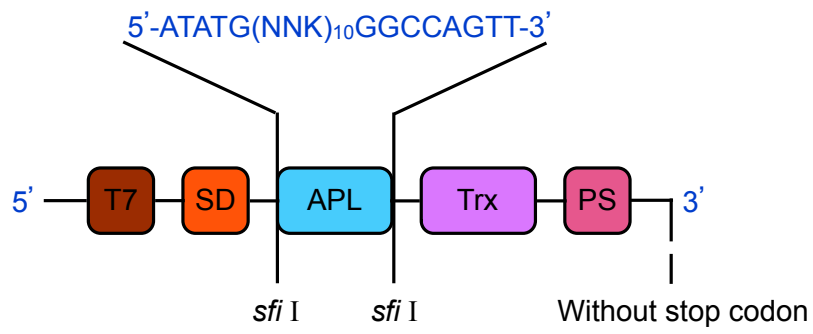
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2 Fig. S1. Structure of DNA libraries.

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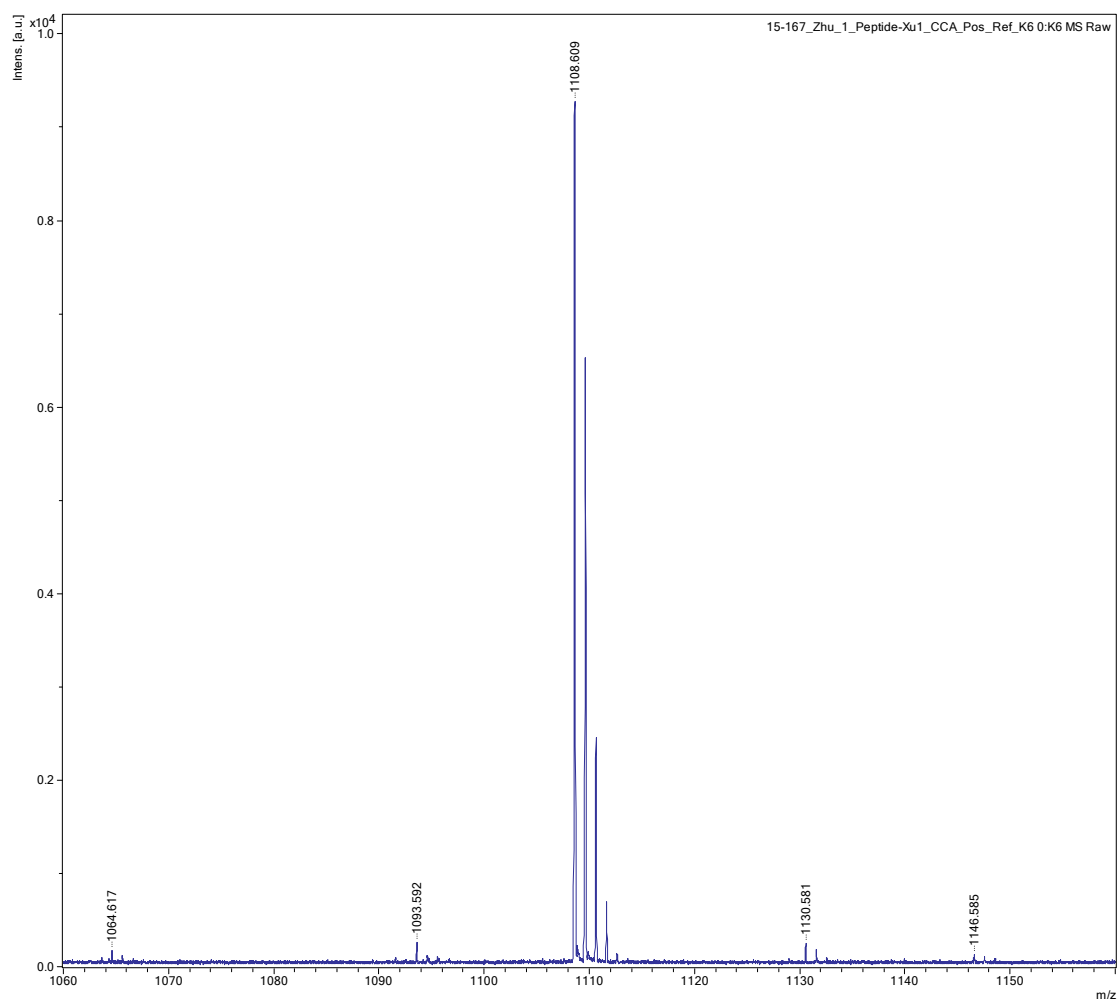
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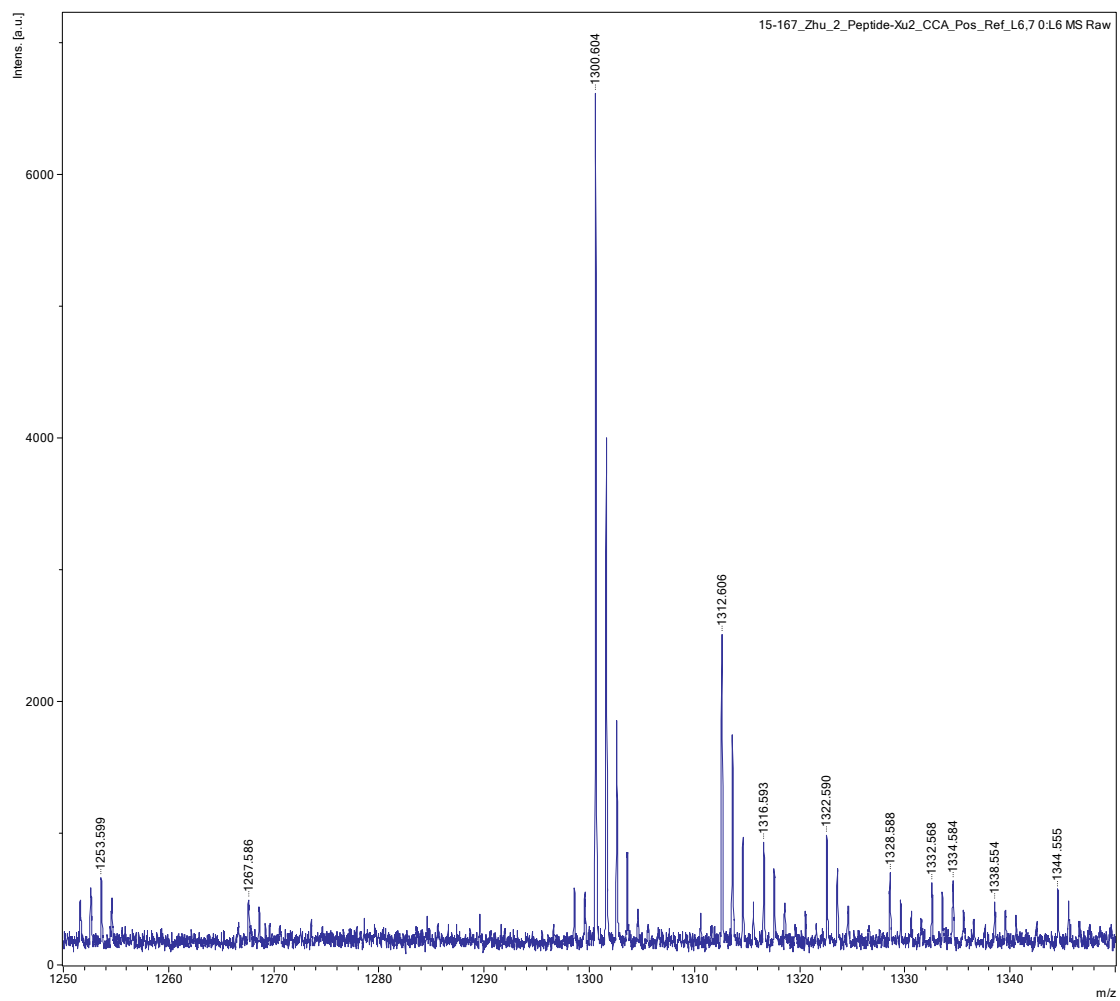
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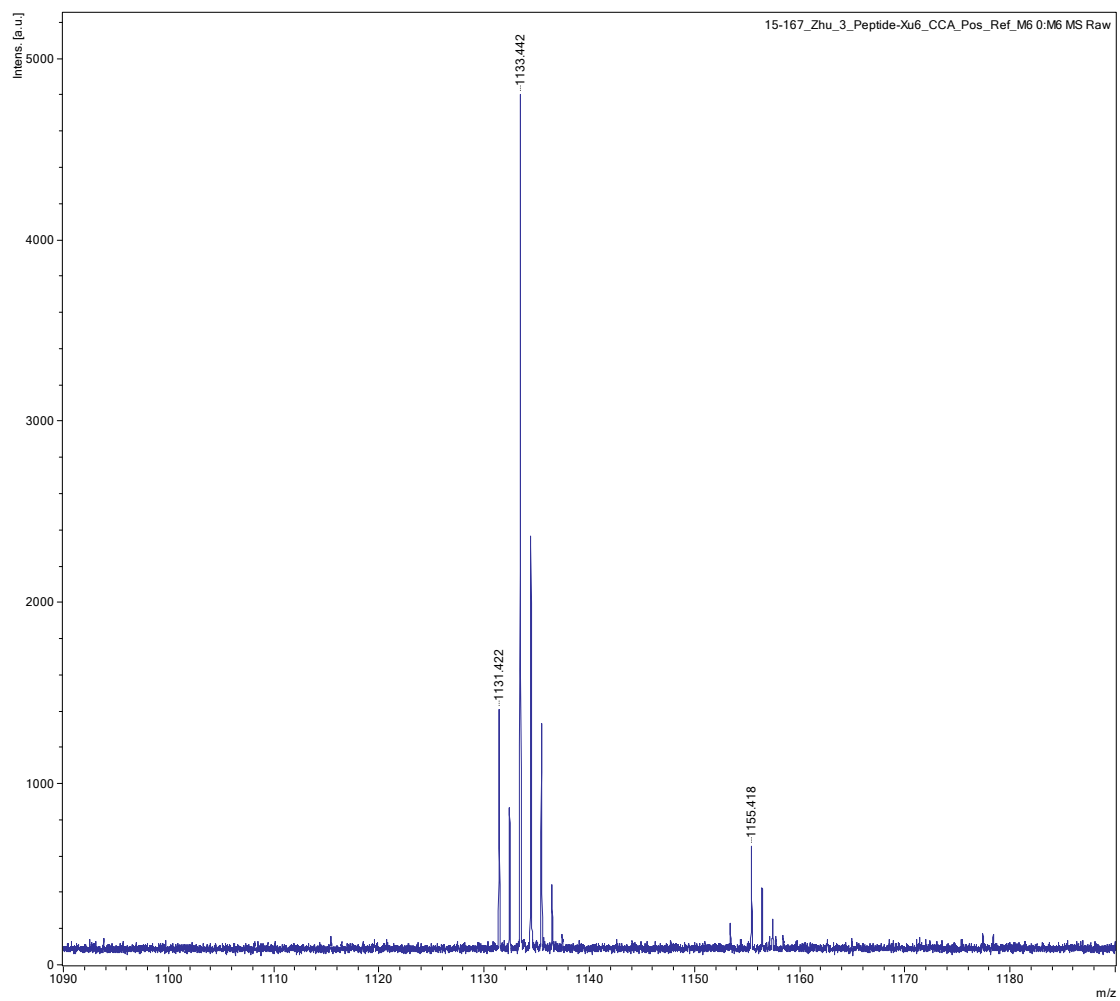
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2 Fig. S2. MALDI-MS spectrum of Xu1 (calcd. for  $C_{52}H_{82}N_{15}O_{12}$   $[M+H]^+$  1108.6,  
3 found 1108.609).



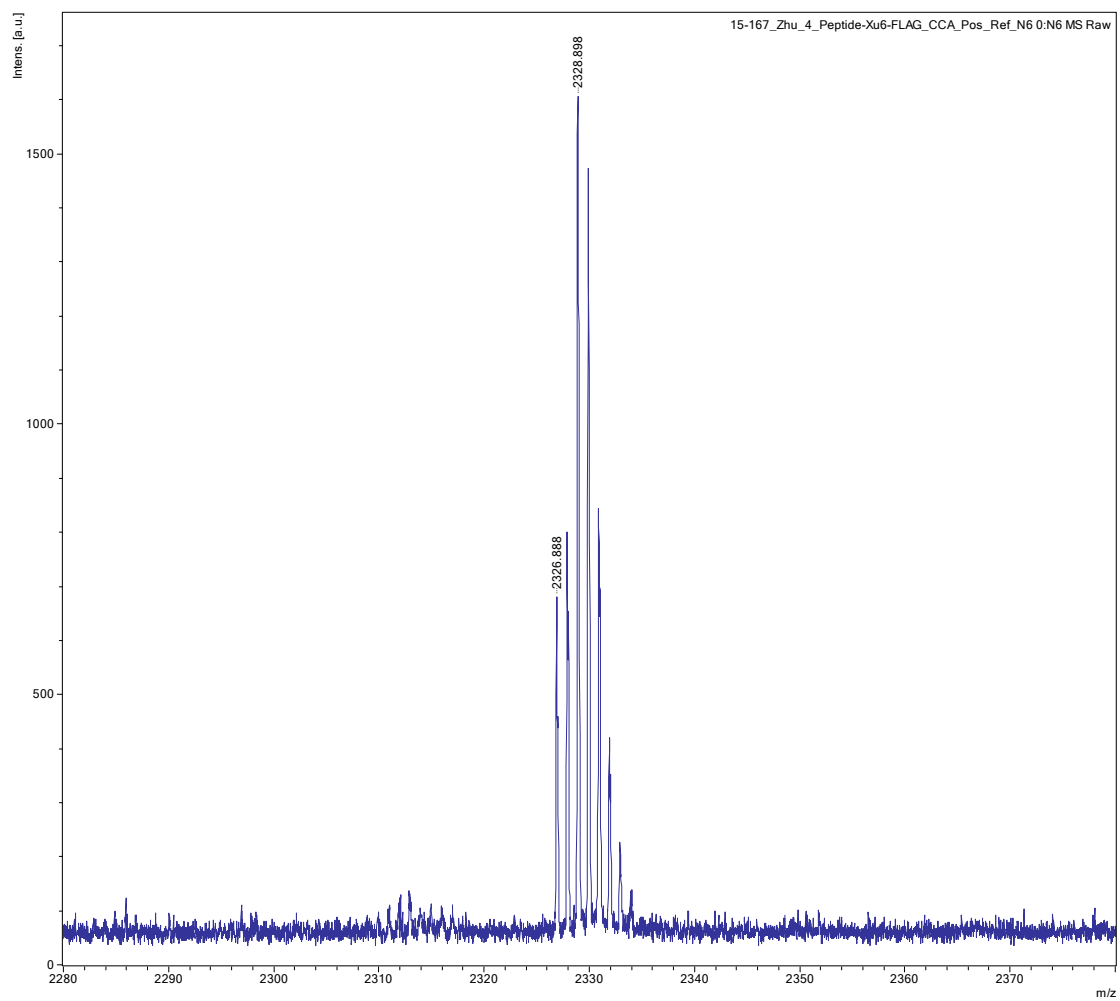
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2 Fig. S3. MALDI-MS spectrum of Xu2 (calcd. for  $C_{63}H_{80}N_{11}O_{16}S [M+Na]^+$  1300.5,  
3 found 1300.604).



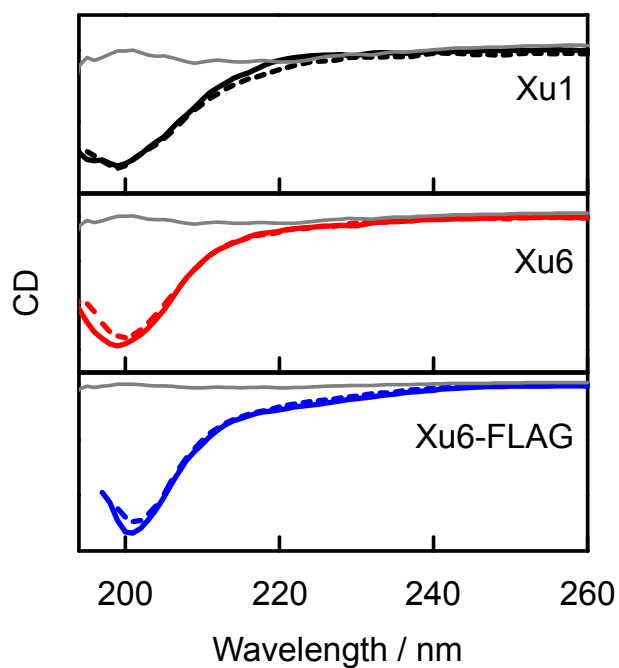
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2 Fig. S4. MALDI-MS spectrum of Xu6 (calcd. for  $C_{43}H_{73}N_{16}O_{16}S_2 [M+H]^+$  1133.5,  
3 found 1133.442).



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2 Fig. S5. MALDI-MS spectrum of Xu6-FLAG (calcd. for  $C_{91}H_{143}N_{30}O_{38}S_2 [M+H]^+$   
3 2329.5, found 2328.898).



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2 Fig. S6. CD spectra of 10 μM of peptide Xu1 (black), Xu6 (red) and Xu6-FLAG (blue)  
3 in the absence (solid line) and presence (dashed line) of 20 μM of hemin in reduced  
4 PBS buffer, where the contributions of hemin alone were subtracted. CD spectra of  
5 20-μM hemin are represented with gray lines.

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Peptide #	Sequence	Peptide #	Sequence	Peptide #	Sequence
01	CLPYCQRYWR	20	LEASILLARF	39	YFTSGLGHVT
02	TLGKCSYSVT	21	SDRHRIDVKL	40	WLTMSSLNS
03	WVVALHWRAK	22	AYDYRFVWAL	41	PFFLIWLSRV
04	MVIPAEFESW	23	CAVVDWFYEF	42	HVSGFELETE
05	CMLSCCAIML	24	FSTLASEFYD	43	CVFPYSTKKL
06	MDNWWDFVNA	25	FTVIYDRFRS	44	DREIEKEALS
07	RLITQFPASL	26	GMSGHGCPQL	45	CYNCQMTSWT
08	YRLPHVVAPG	27	PEAYCILWYL	46	YCGSYDSHTL
09	YSSPKWNALL	28	IVVAPRSERK	47	VRVVVIKMM
10	FLCLCSSLLS	29	YCLFCVDFG	48	FLAGLSETFF
11	RMLQVMYFMR	30	DLVATSVFWW	49	YGSTYLSGML
12	ISYVHVYLDL	31	LPYEHLHCK	50	SLTAEFSYSR
13	CAVVDWFYEF	32	GMLITMRLEL	51	SAECTRQCH
14	ALSVLPERQG	33	AESVEASKFY	52	LPTRHTARTQ
15	ELMGGGDYKD	34	FRQAETTCHF	53	LEVTLAPNV
16	MLVVVVIKIM	35	SLMRHMGDKV	54	MVISFDLGCL
17	VFHLVIPTLL	36	LLRPMSDTWL	55	MEDRWNDEKP
18	MISWFQWLLG	37	LVCYLSRLQS	56	RLMVSKLWTR
19	AMKVLRLNSW	38	CSWLRSMSKP	57	ICSGRADSKL

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2 Table S1. Sequence list of selected peptides.