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Supplementary Materials for

A new algorithm to convert a normal antibody into the corresponding catalytic antibody

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Fig. S1. Mass spectroscopy.

Table S1. Distances between two amino acid residues.

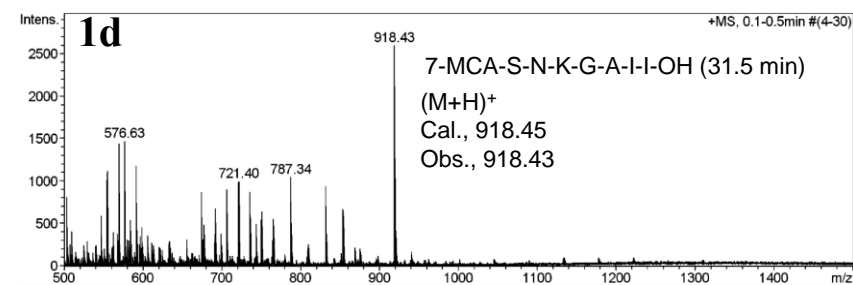
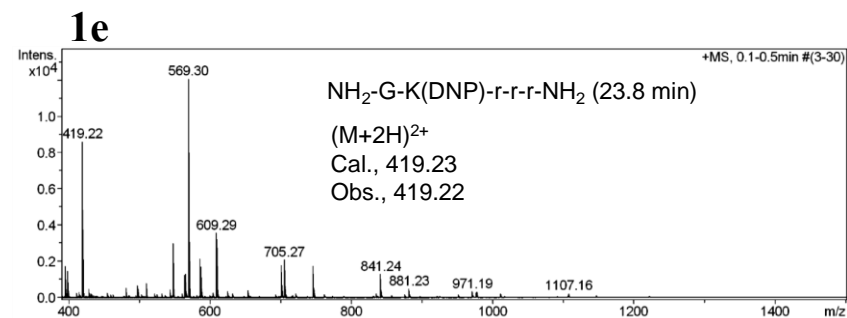
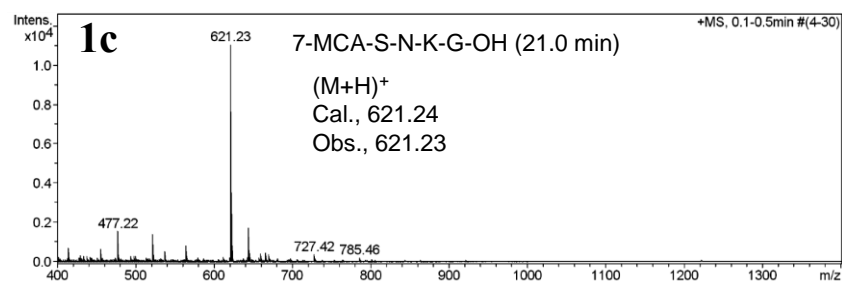
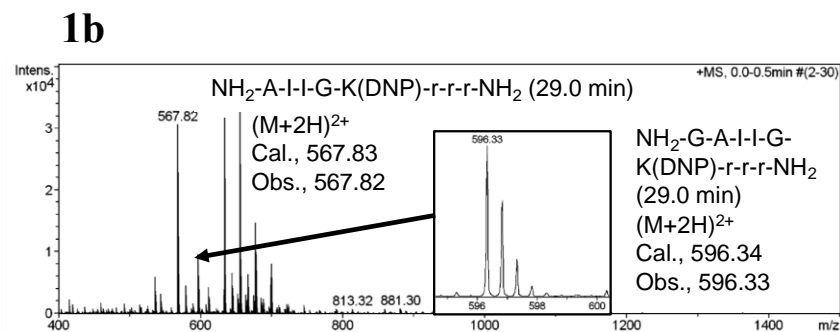
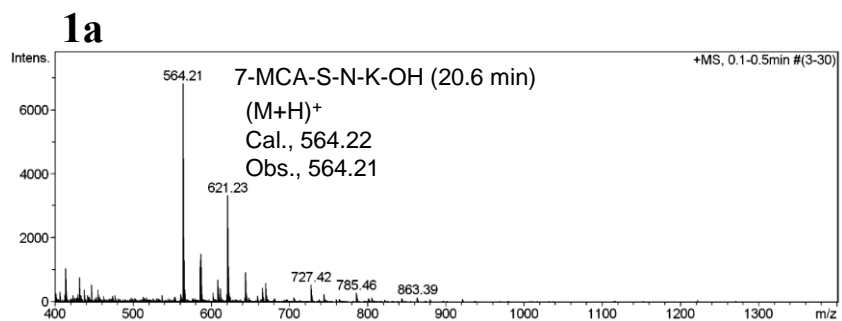


Fig. S1a-1e

Fig. S1. Mass spectroscopy. The fragmented peptides observed in HPLC were identified by mass spectroscopy analysis. For the peaks of 7-MCA-S-N-K-OH (20.6 min) and NH₂-G-A-I-I-G-K(DNP)-r-r-r-NH₂ (29 min), the monovalent mass was detected at 564.22 m/z (Fig. 1a) and the divalent mass at 596.34 $m/2z$ (Fig. 1b: inset graph), respectively. For the fragments of 7-MCA-S-N-K-G-OH (21 min) and NH₂-A-I-I-G-K(DNP)-r-r-r-NH₂ (29 min), the monovalent mass was observed at 621.24 m/z (Fig. 1c) and the divalent at 567.83 $m/2z$ (Fig. 1b), respectively. For the peaks of 7-MCA-S-N-K-G-A-I-I-OH (31.5min) and NH₂-G-K(DNP)-r-r-r-NH₂ (23.8 min), the monovalent mass was detected at 918.45 $m/2z$ (Fig. 1d) and the divalent at 419.23 $m/2z$ (Fig. 1e), respectively.

Table S1. Distances between two amino acid residues.

Table S1 Distances between two amino acid residues

	Distances between functional groups (Å)	
Light chain	Ser27a(O)-His27d(N)	His27d(O)-Asp1(O)
S35	10.37	17.42
S38	10.43	13.77
Light chain	Ser27a(O)-His93(N)	His93(O)-Asp1(O)
T99wt	7.46	12.26
T99 Pro95(-)	6.20	6.21