

Supplementary Information for

## **Elucidation of inhibitor-binding pocket of D-amino acid oxidase using docking simulation and *N*-sulfanylethylanilide-based labeling technology**

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E-mail:

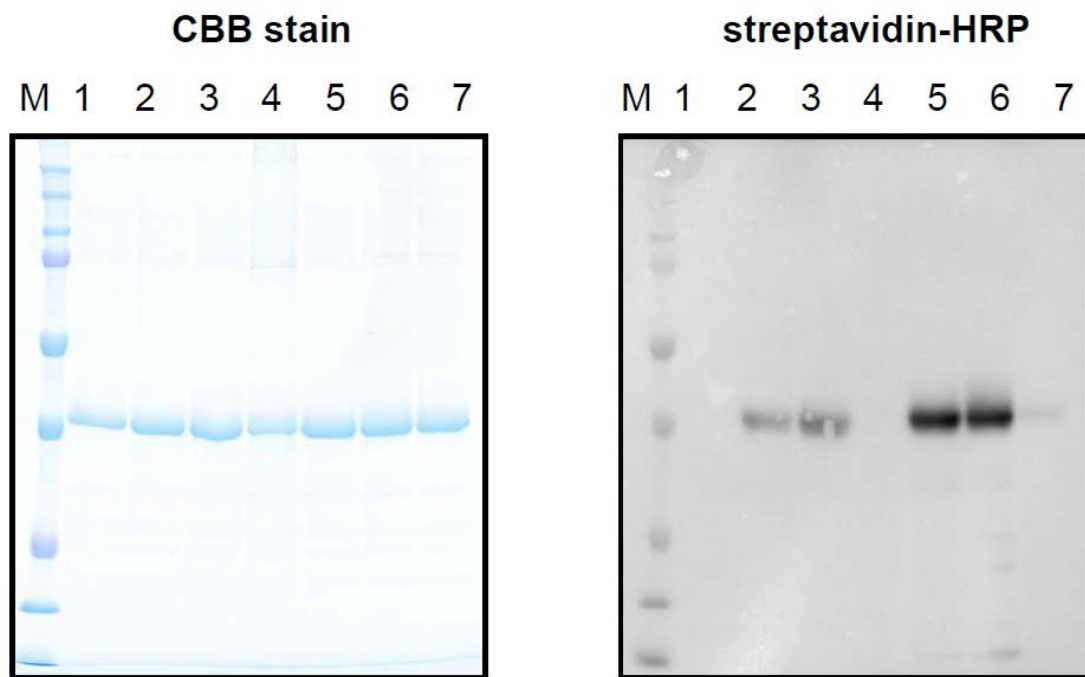
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kiyo.fukui@tokushima-u.ac.jp (K. Fukui)

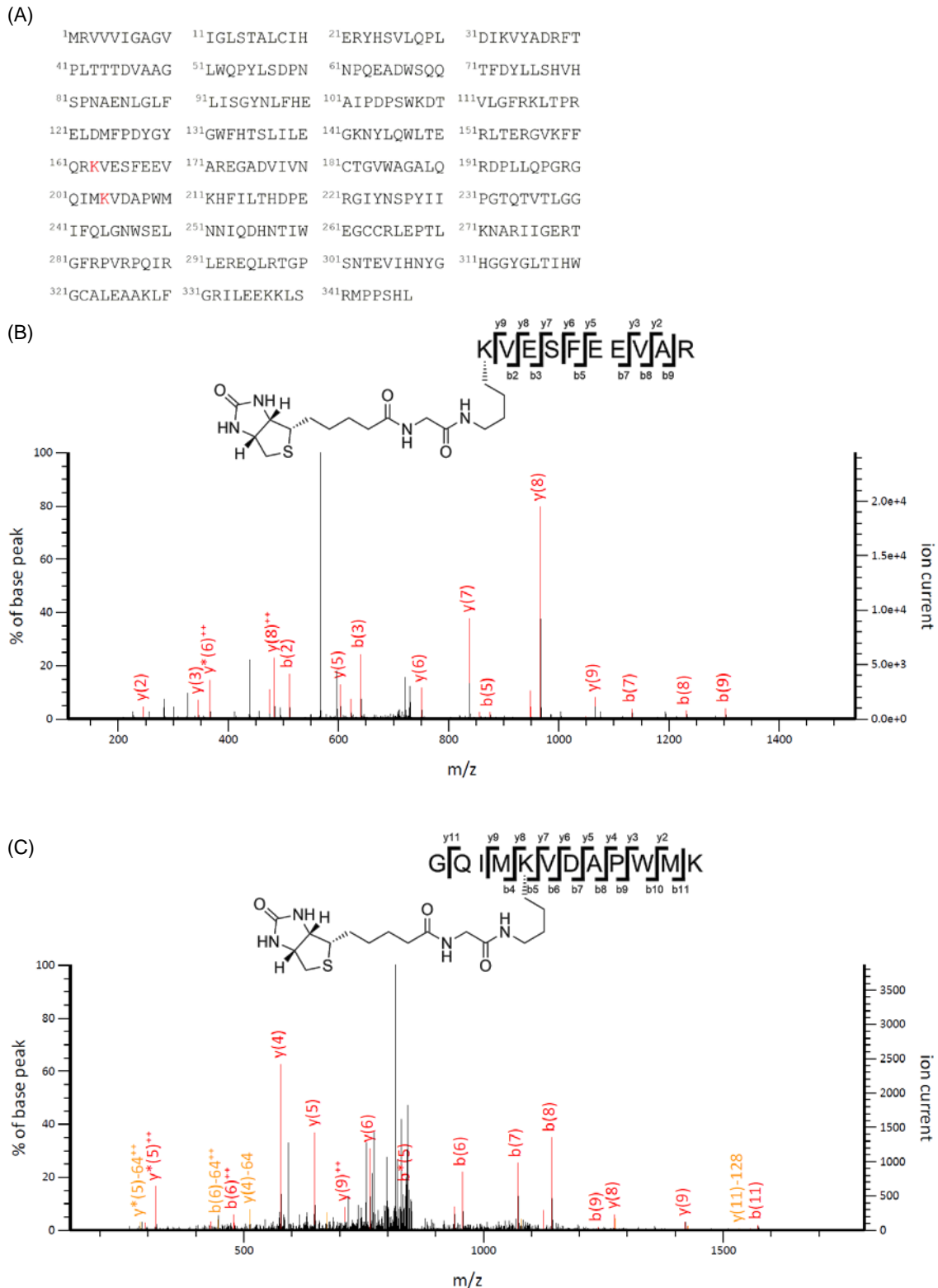
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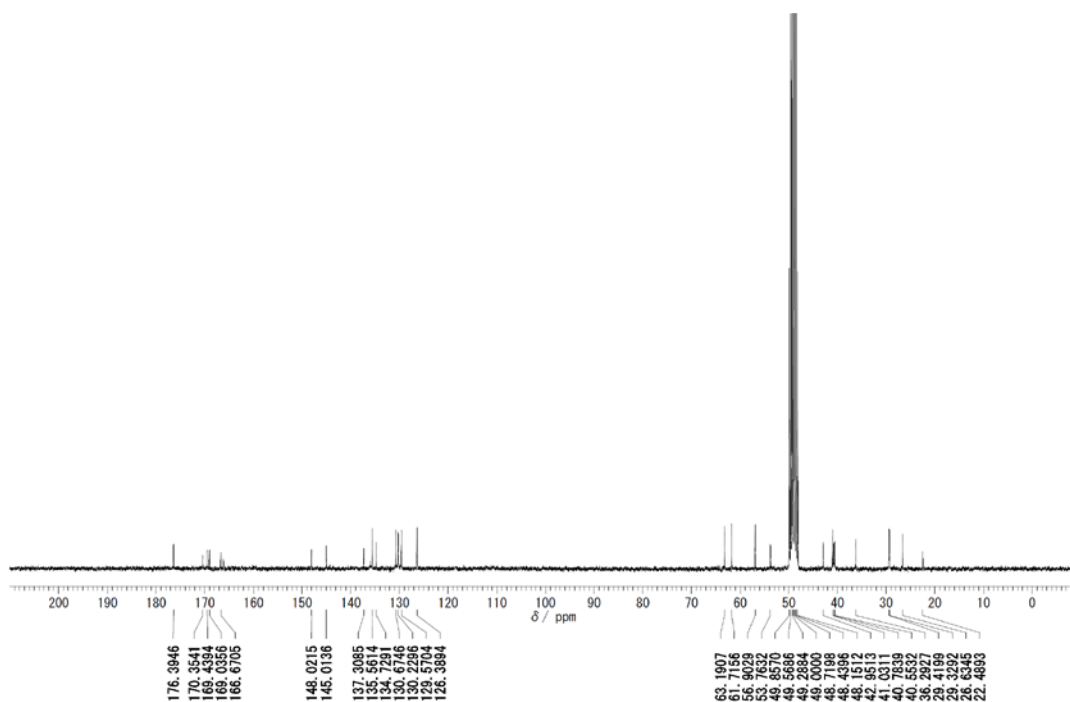
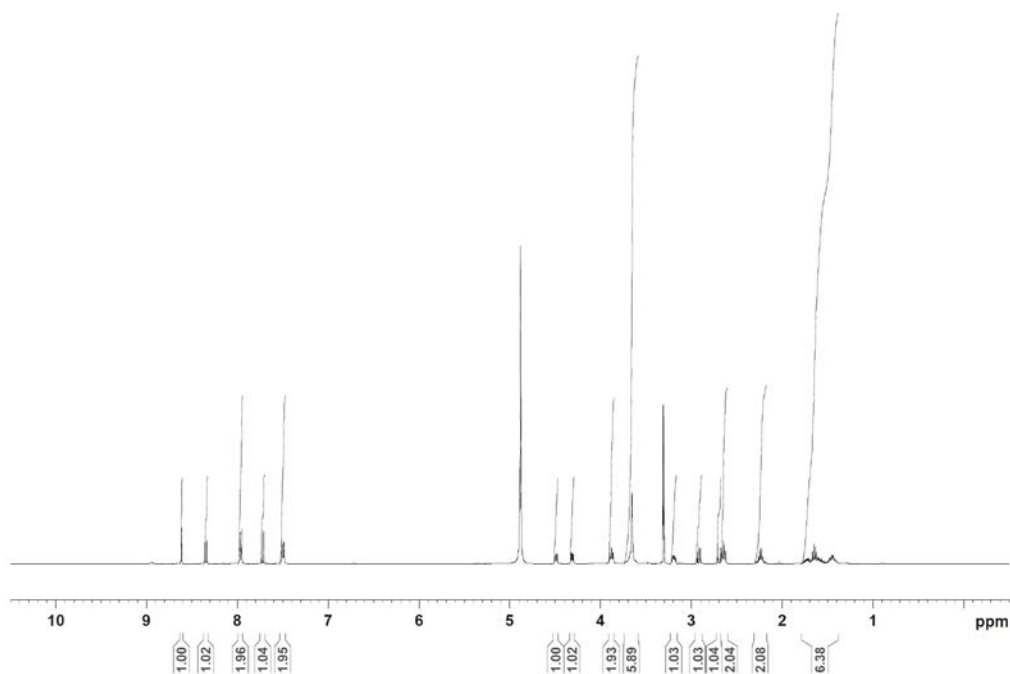
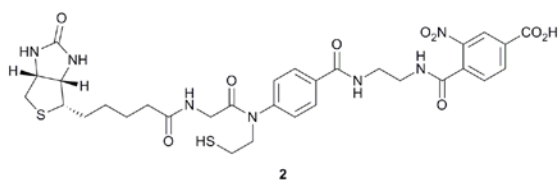
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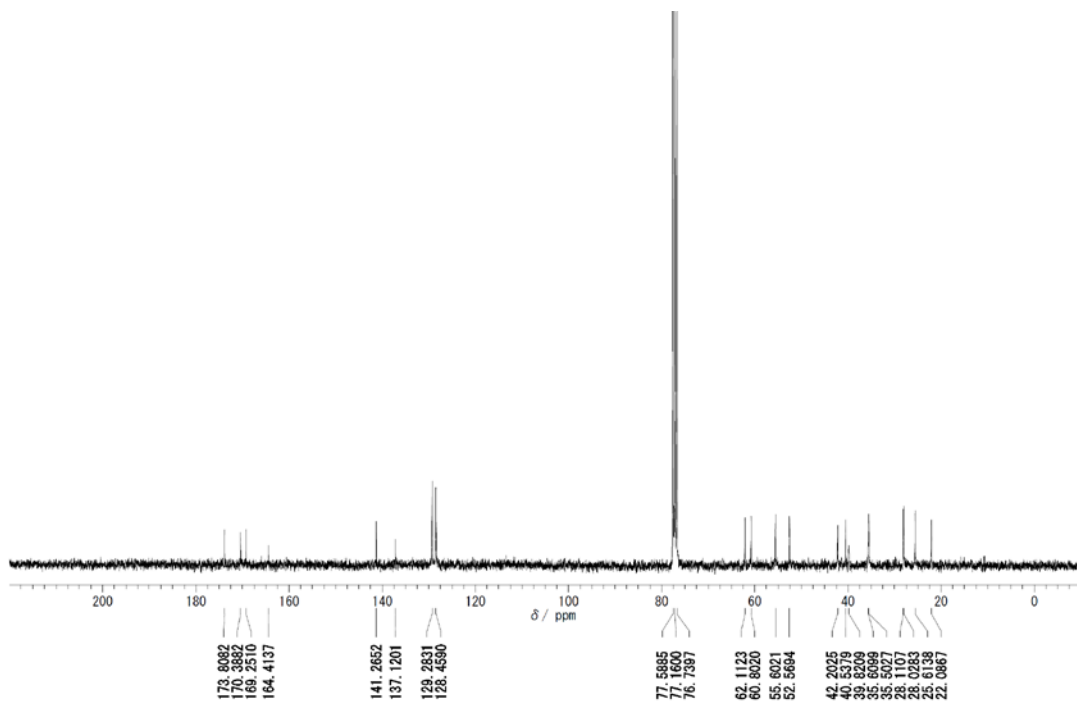
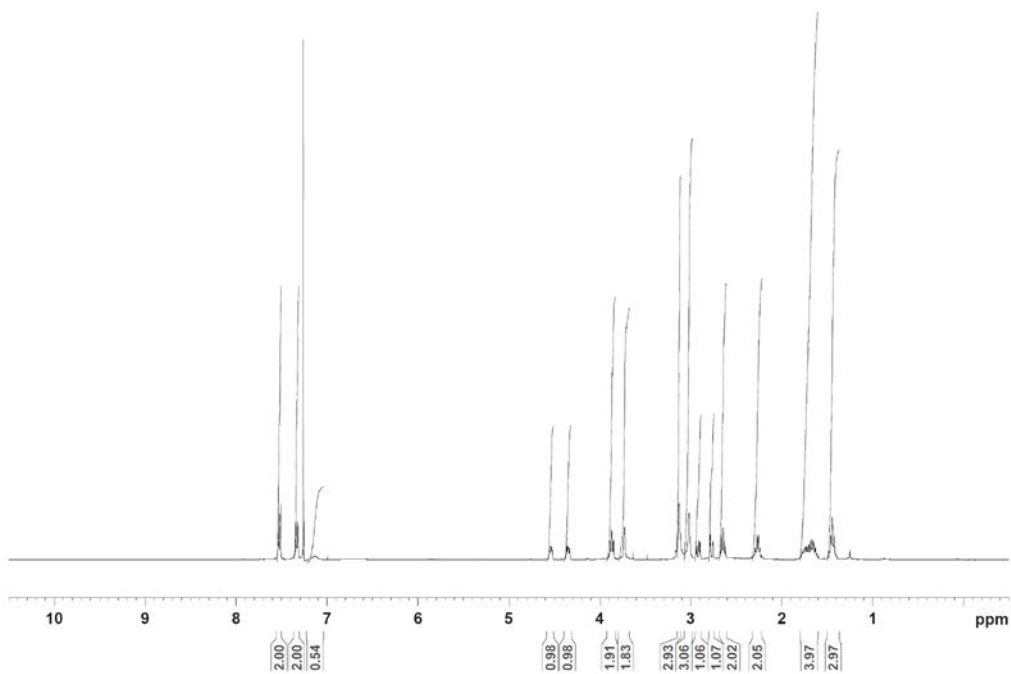
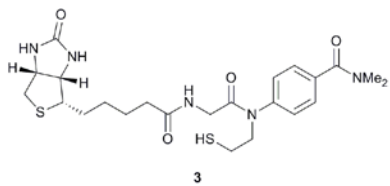


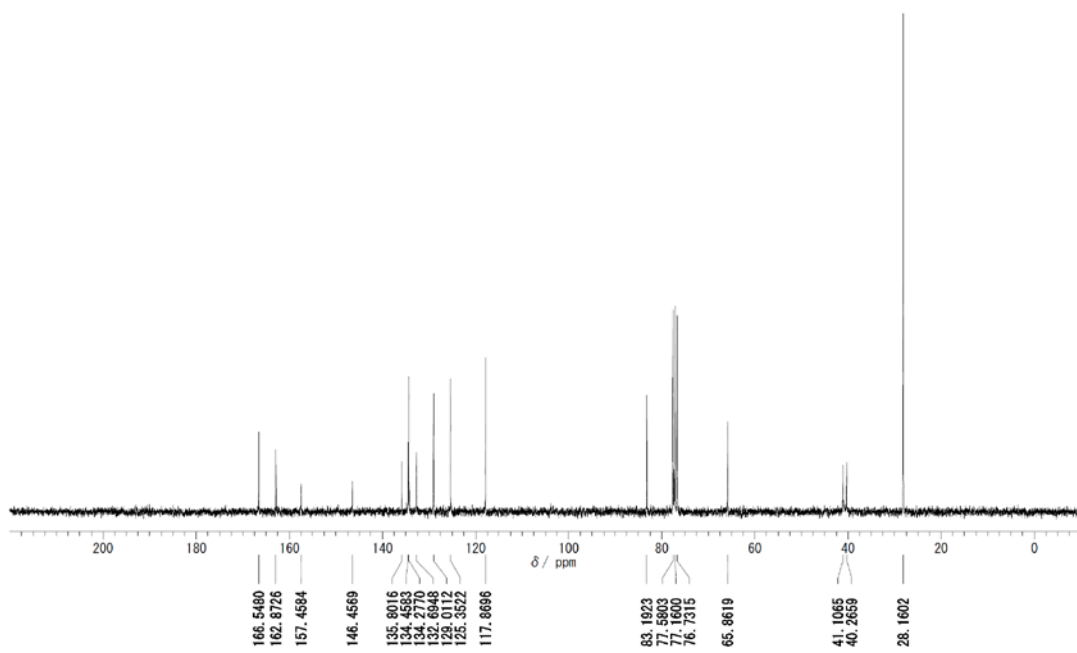
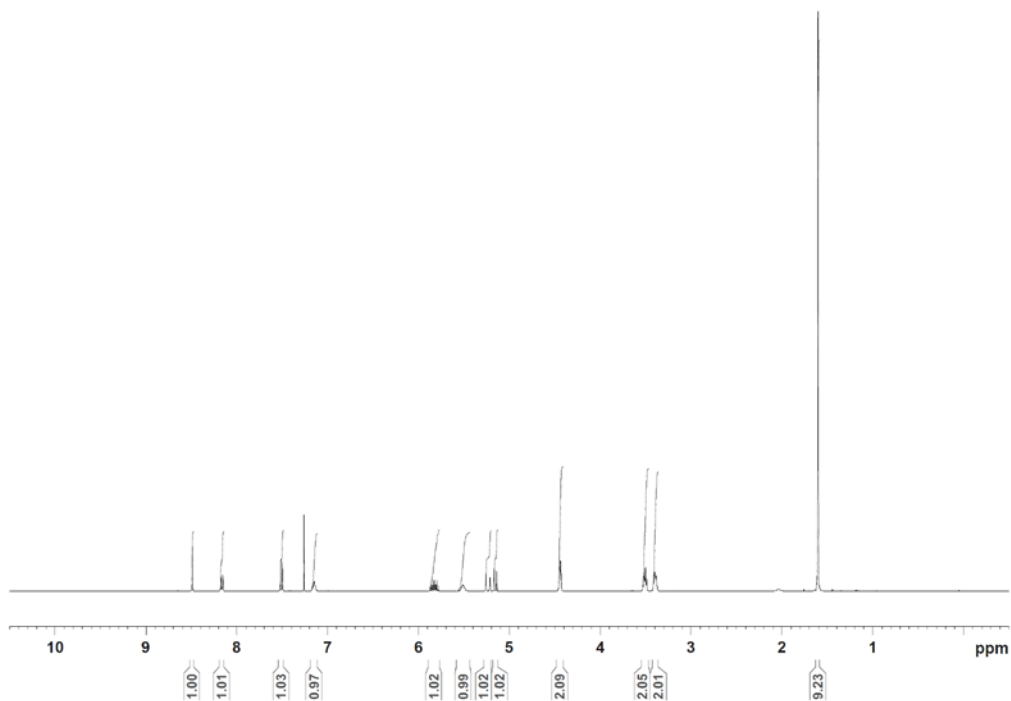
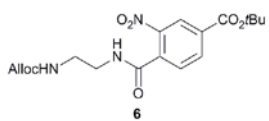
**Fig. S1** An original picture of Fig. 4C. Lane 4 and 7 in Fig. S1 correspond to lane 1 and 2 in Fig. 4C, respectively.

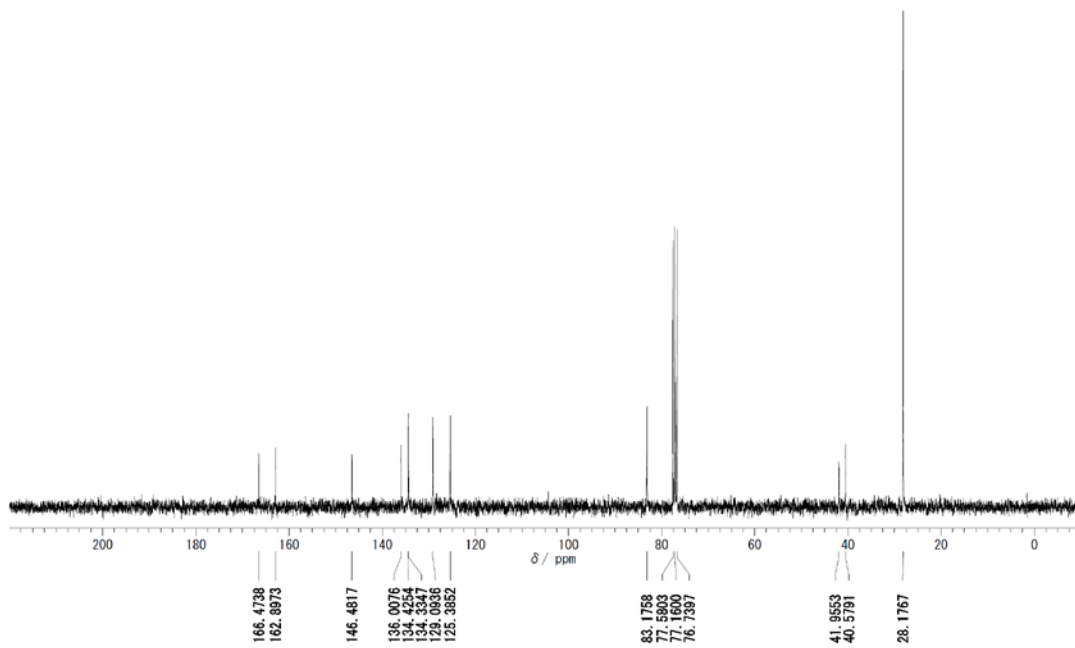
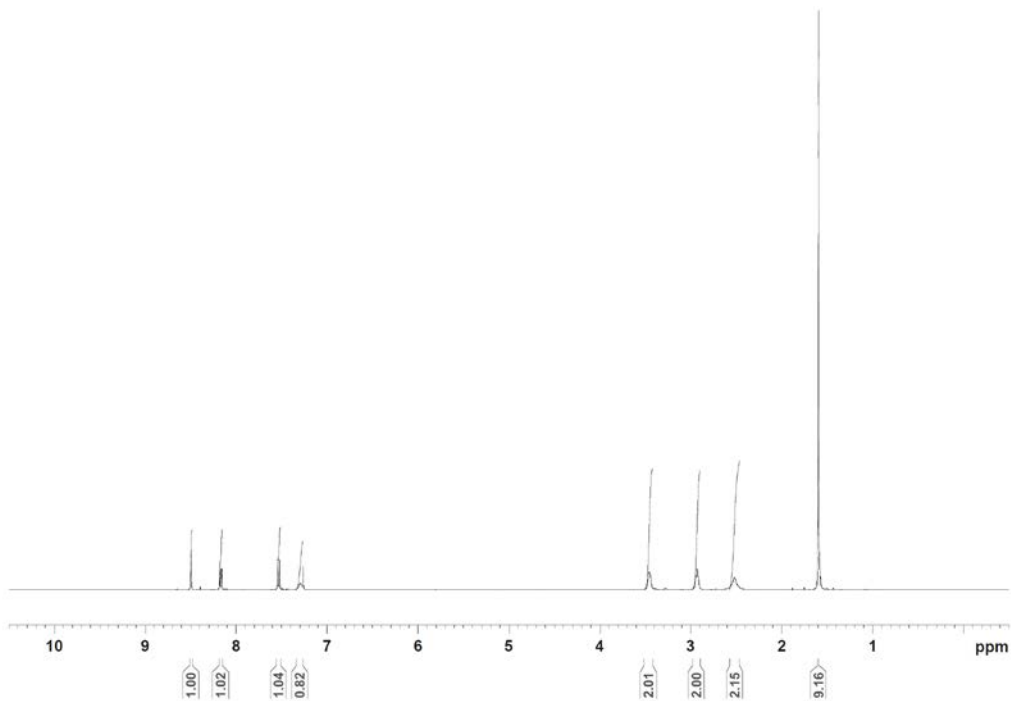
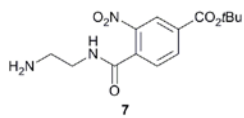


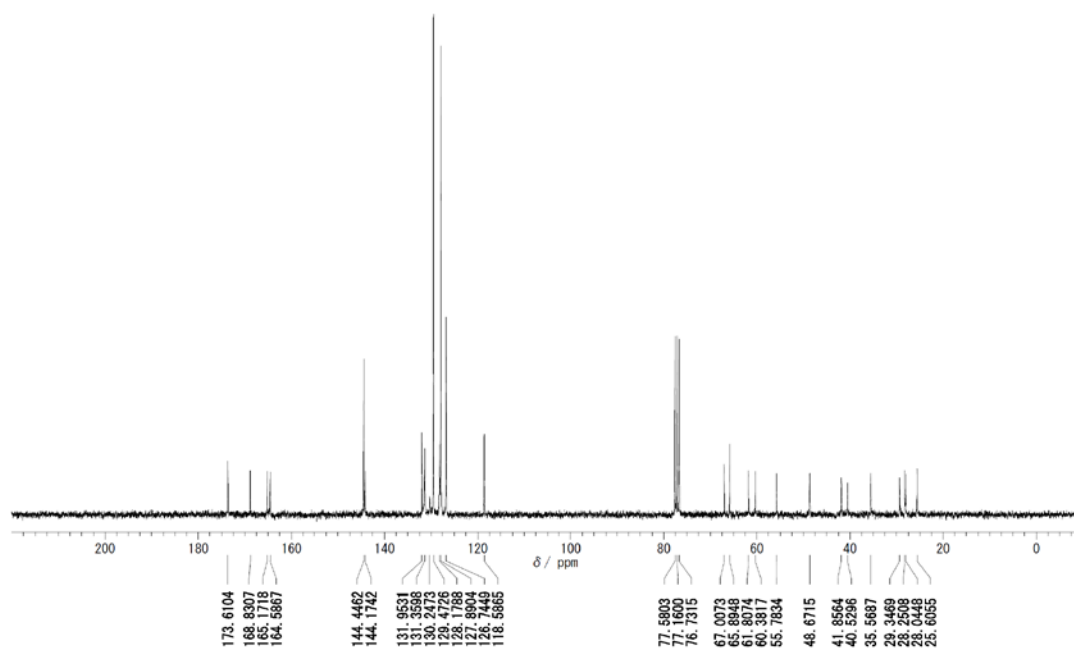
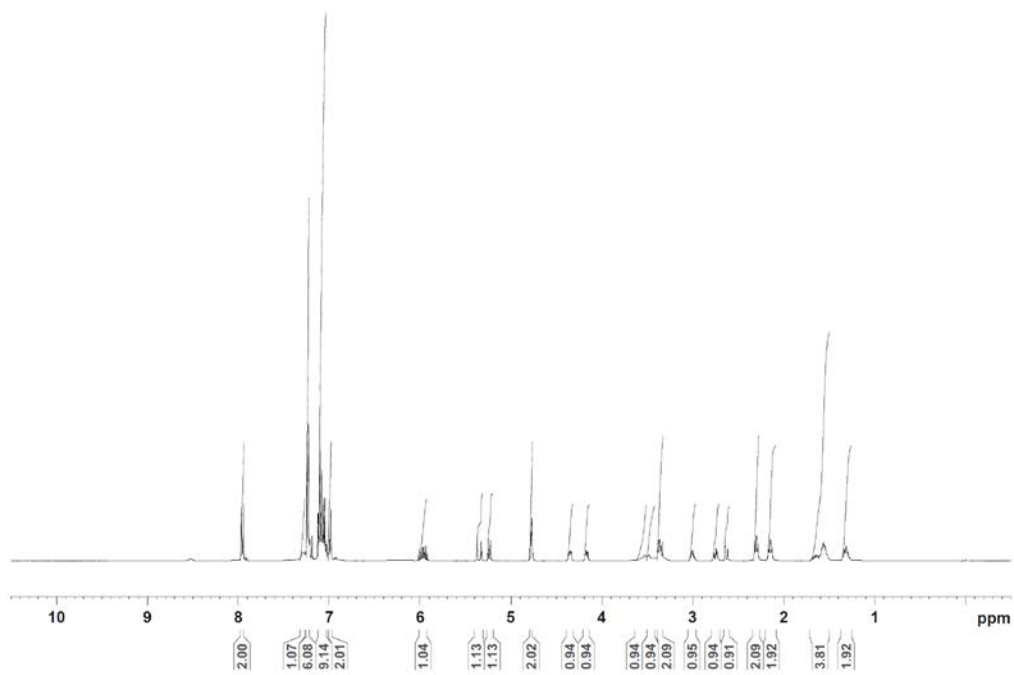
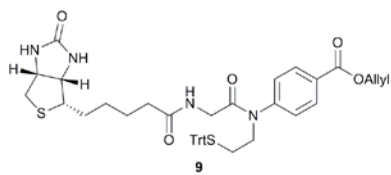
**Fig. S2** Mass spectral analysis of the labeled residues of DAO using SEAL reagent 2. (A) A primary sequence of DAO. (B and C) nanoLC-MS/MS analysis of the fragments labeled at Lys163 (B) and 204 (C).



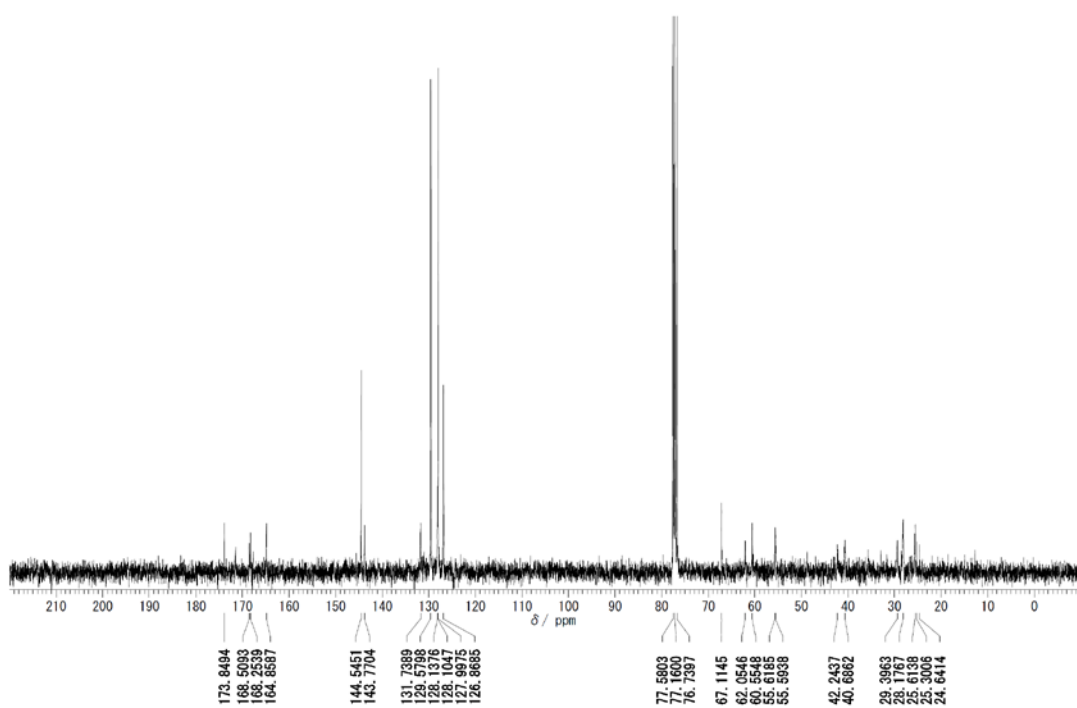
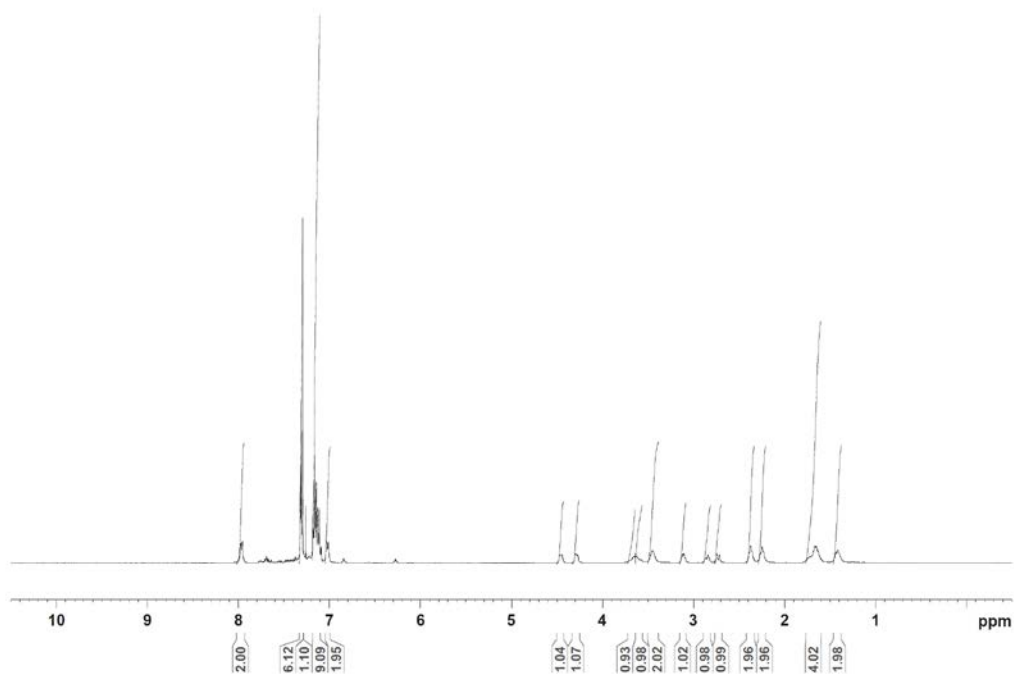
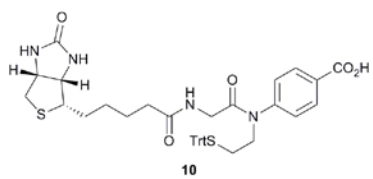


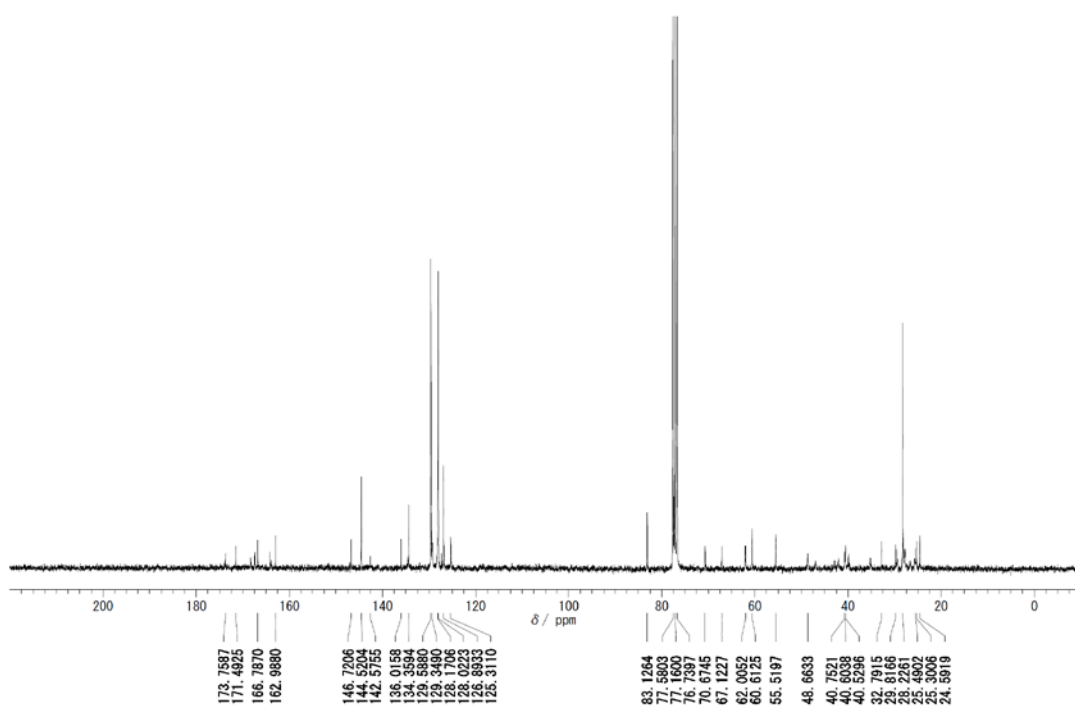
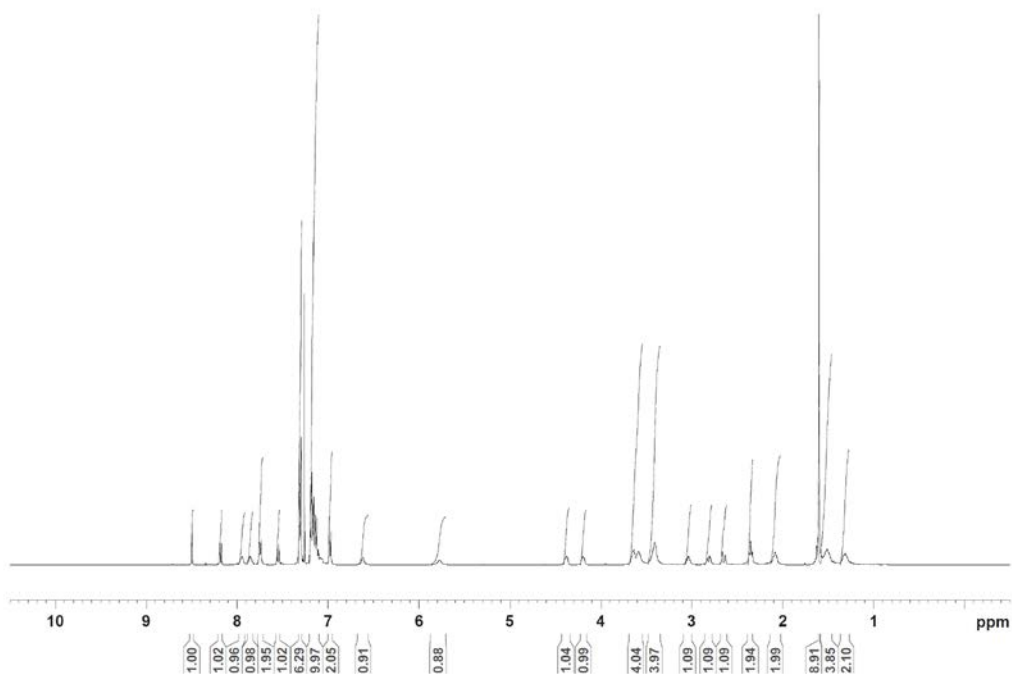
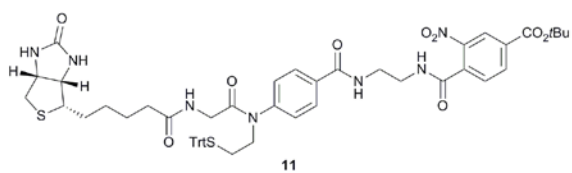


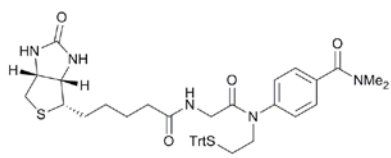












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