

## Supporting Information

### Design of the coiled-coil N-peptide against HIV-1 based on the CADD strategy

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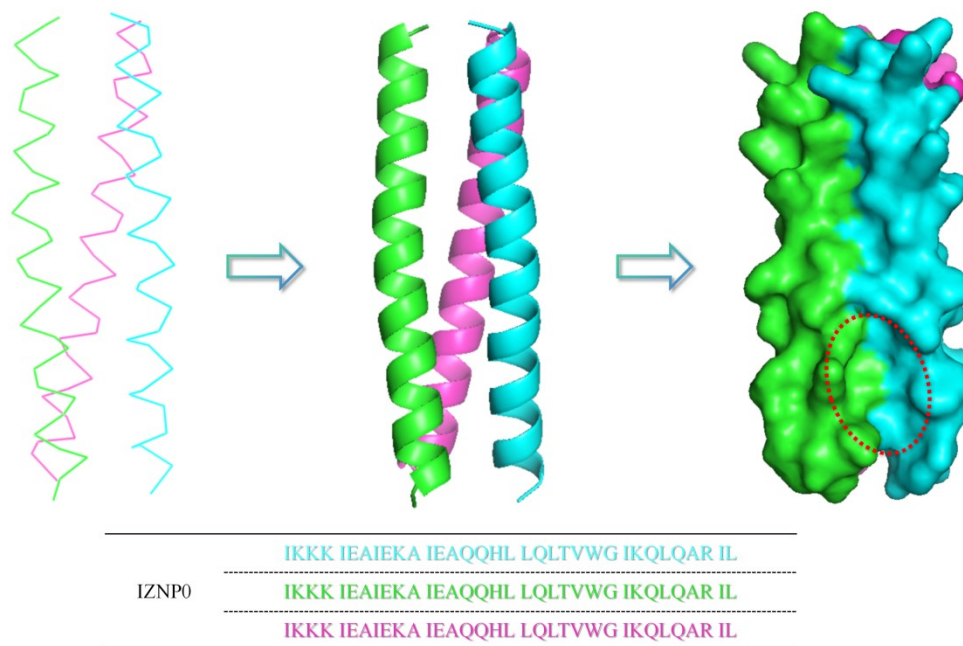
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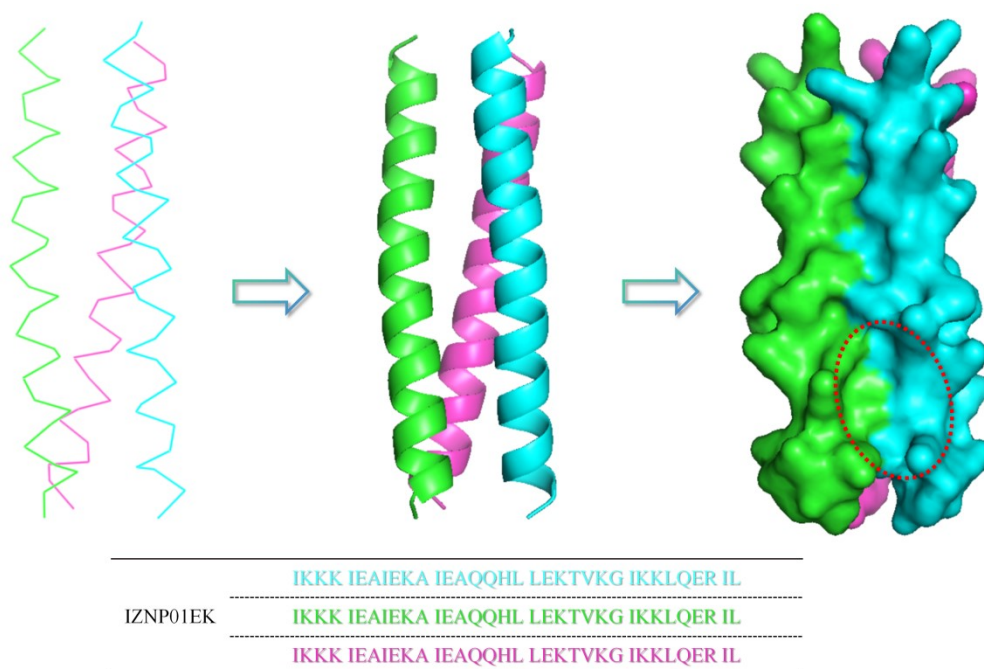
# These authors contributed equally to this work.

Content:

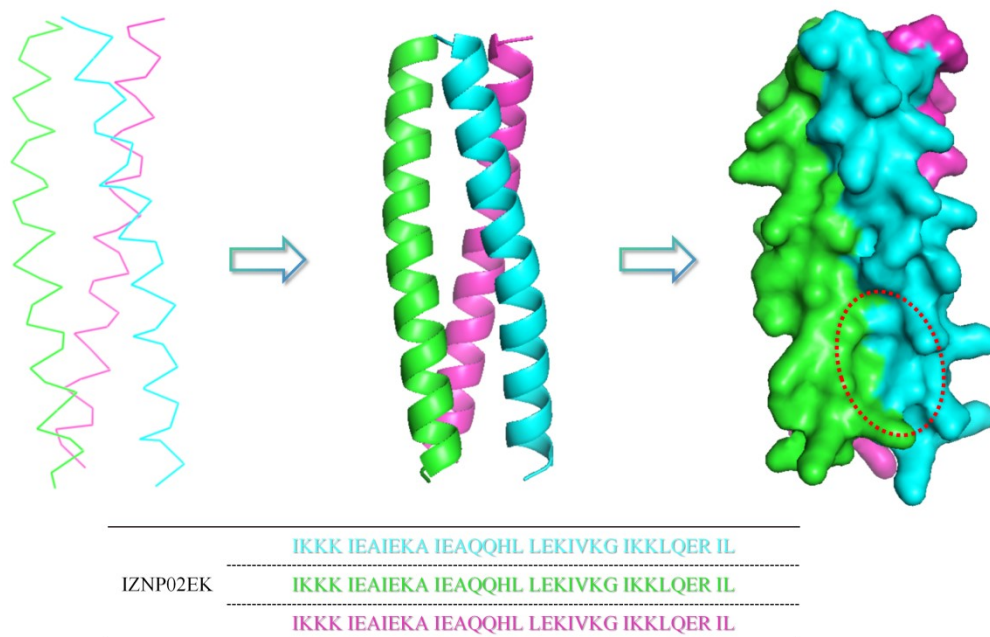
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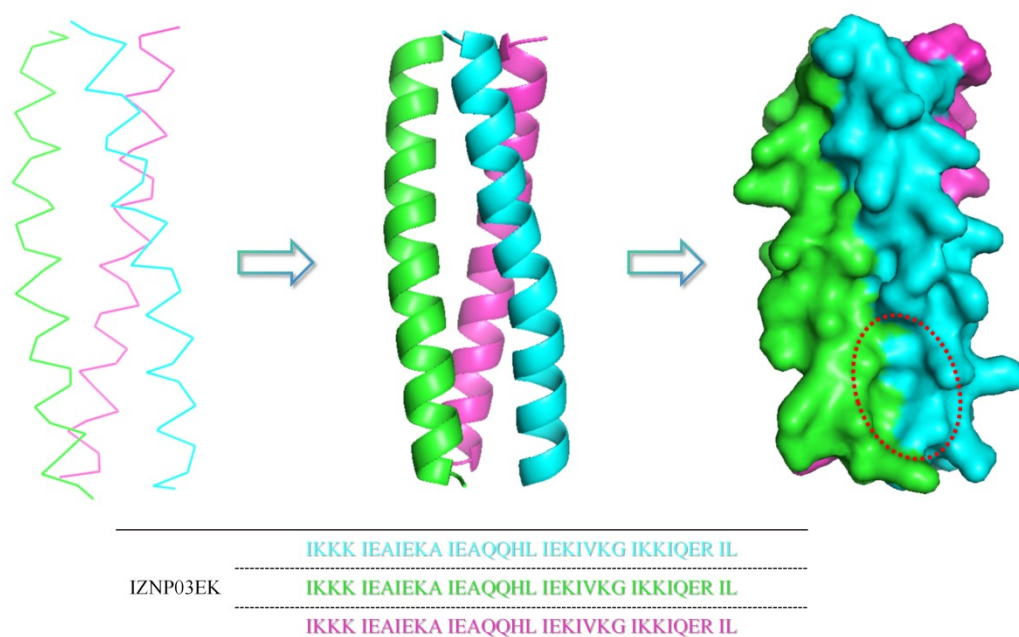
**Figure S1.** The triple helix conformation of IZNP0 is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



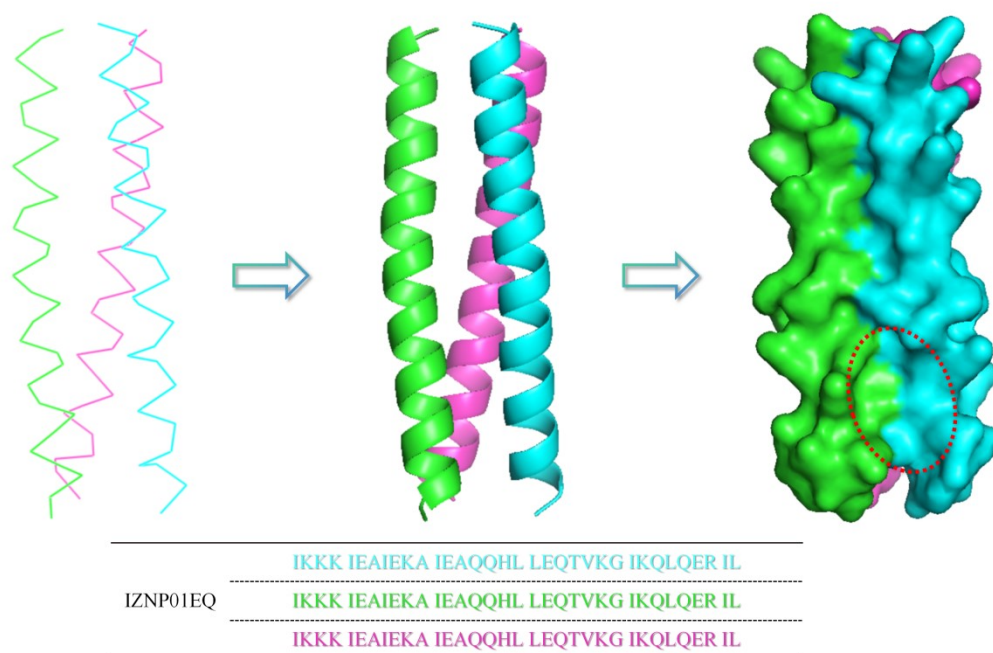
**Figure S2.** The triple helix conformation of IZNP01EK is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



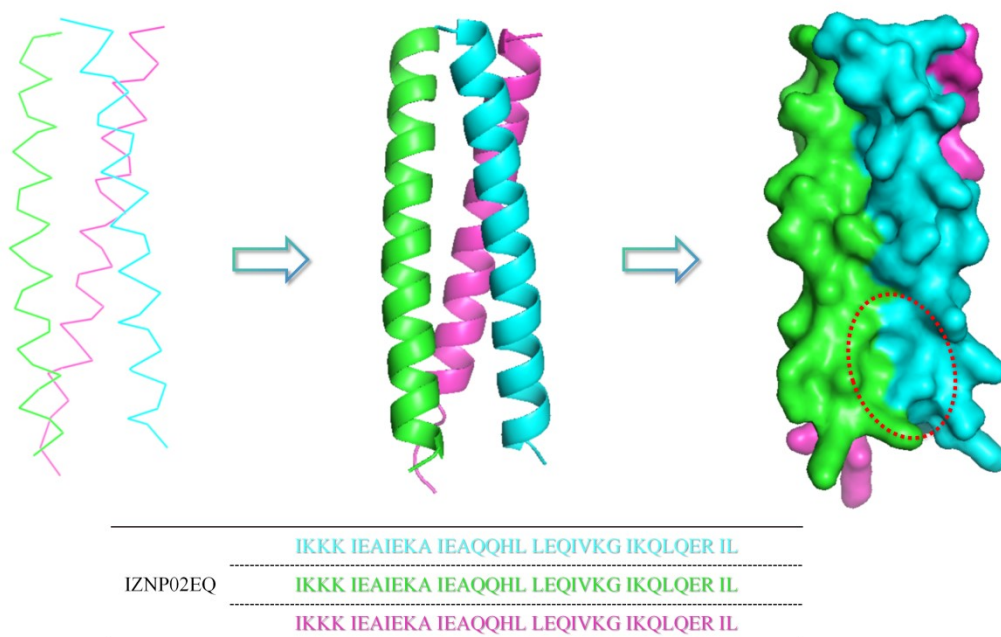
**Figure S3.** The triple helix conformation of IZNP02EK is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



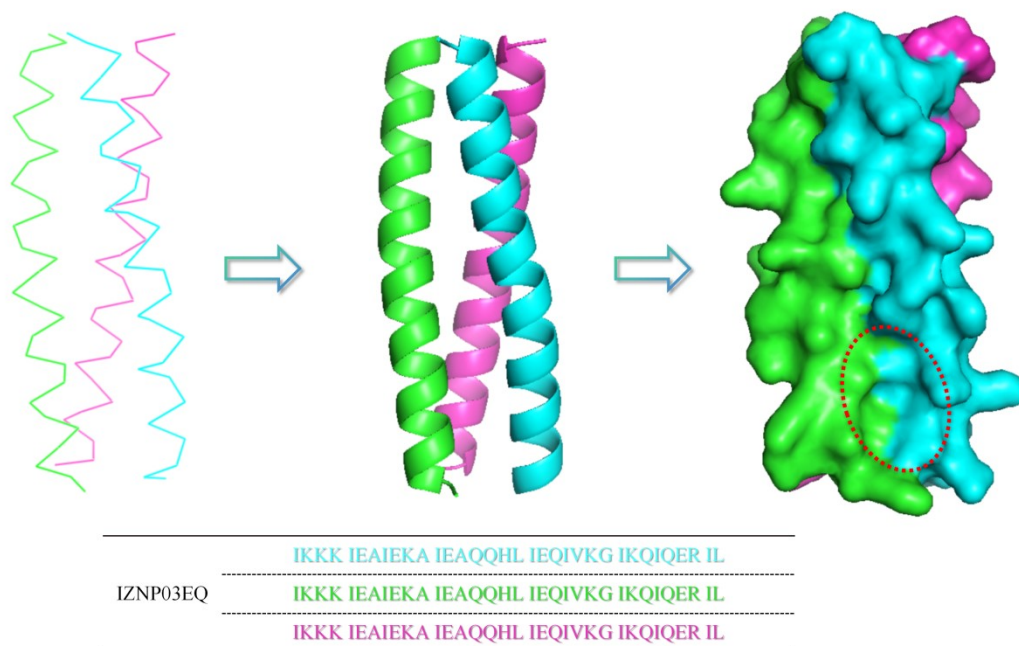
**Figure S4.** The triple helix conformation of IZNP03EK is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



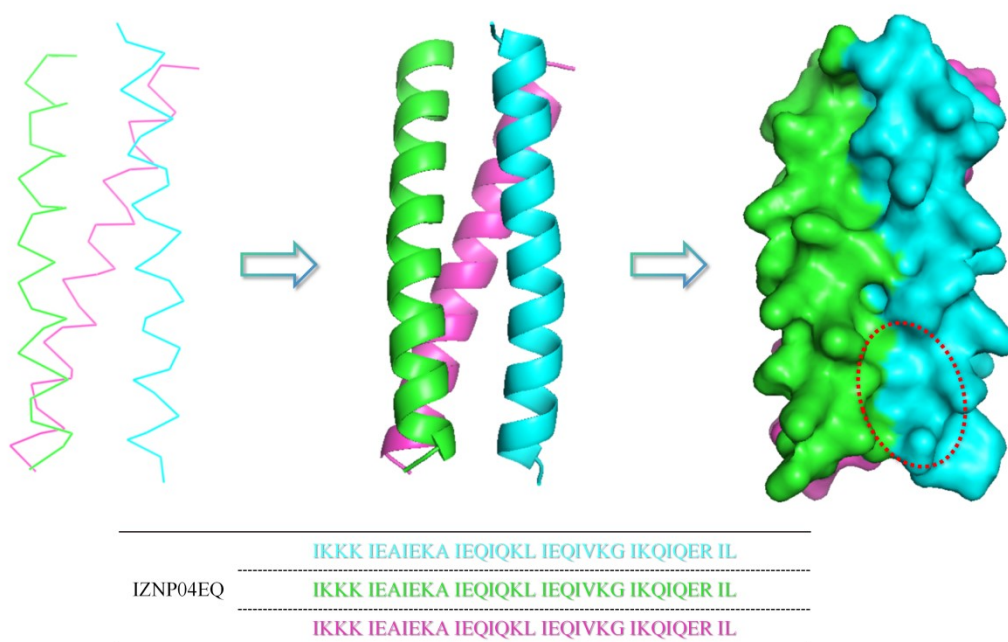
**Figure S5.** The triple helix conformation of IZNP01EQ is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



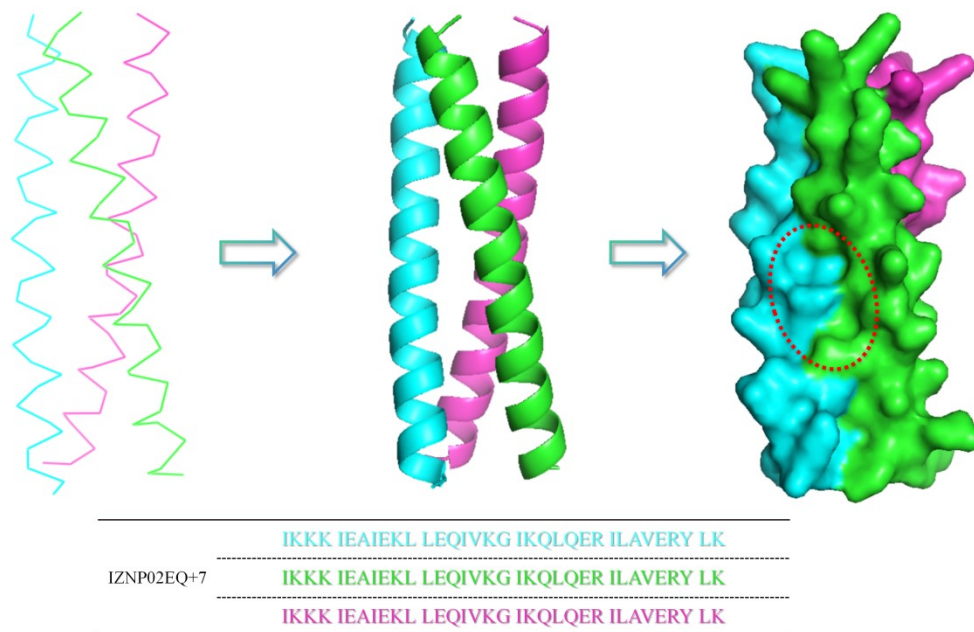
**Figure S6.** The triple helix conformation of IZNP02EQ is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



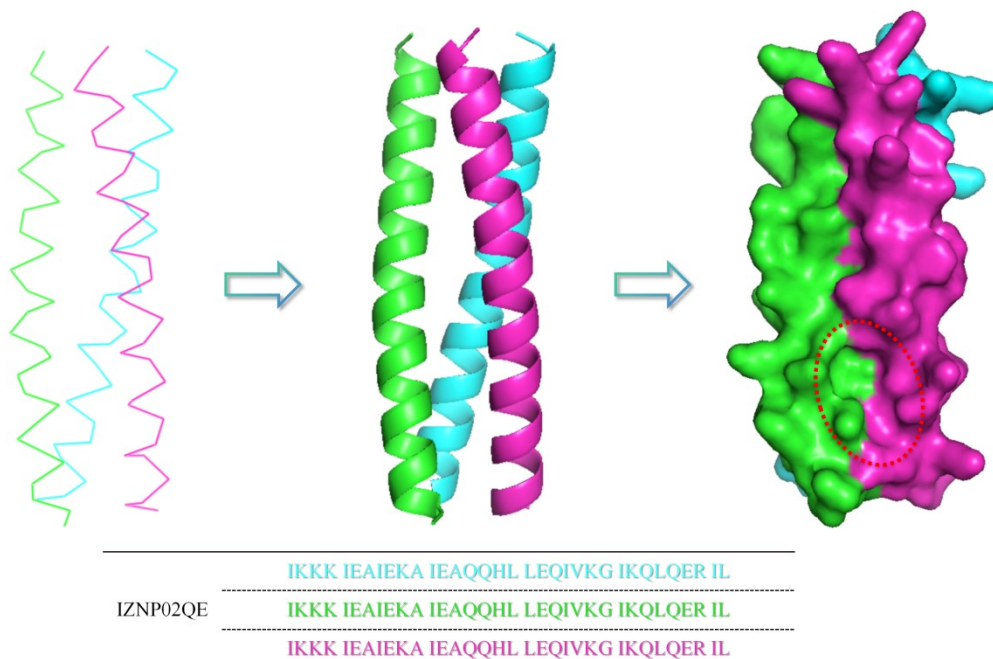
**Figure S7.** The triple helix conformation of IZNP03EQ is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



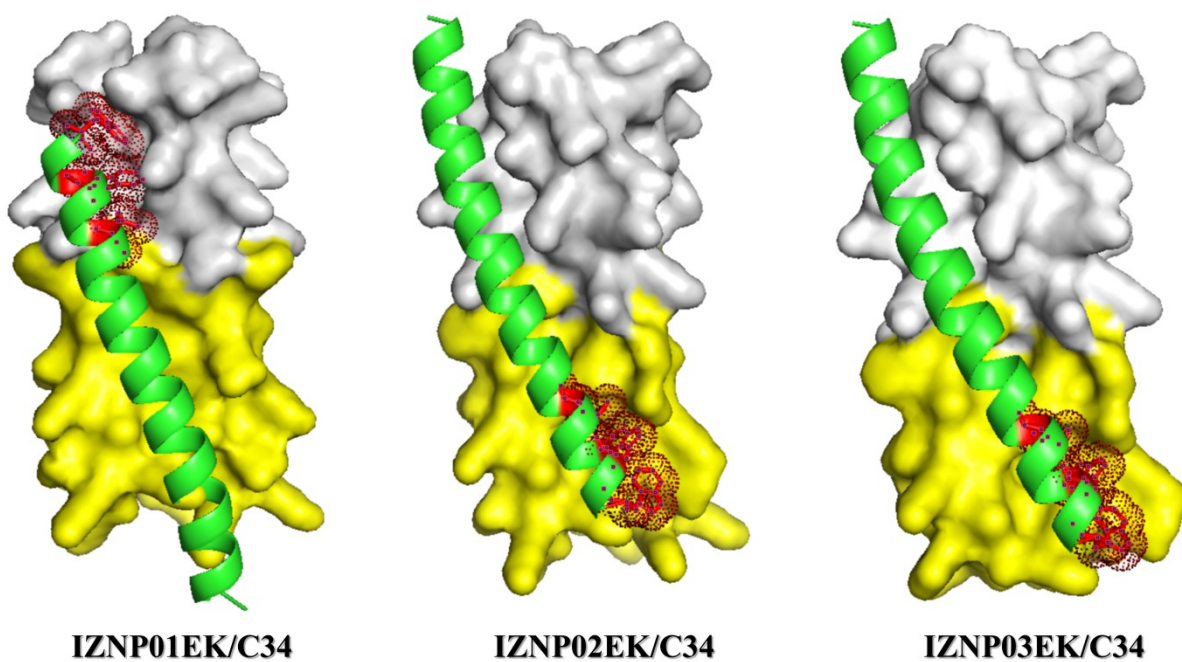
**Figure S8.** The triple helix conformation of IZNP04EQ is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



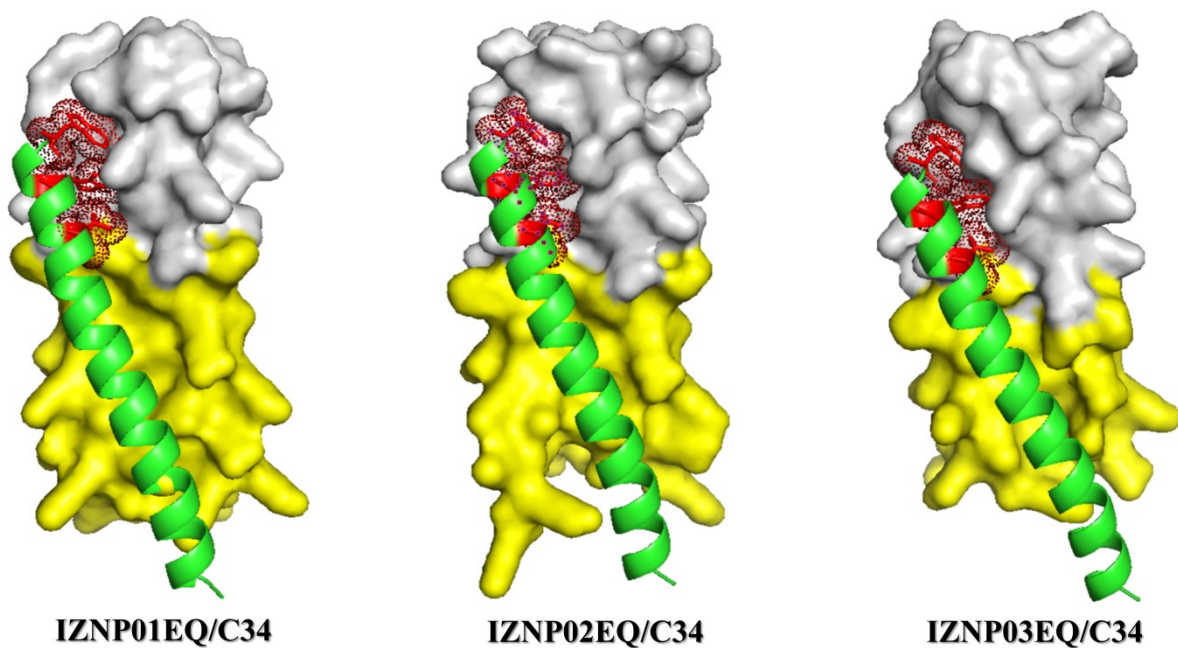
**Figure S9.** The triple helix conformation of IZNP02EQ+7 is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".



**Figure S10.** The triple helix conformation of IZNP02QE is shown in ribbon, cartoon representation and electrostatic surface. The dashed red circle represents the "Pocket domain".

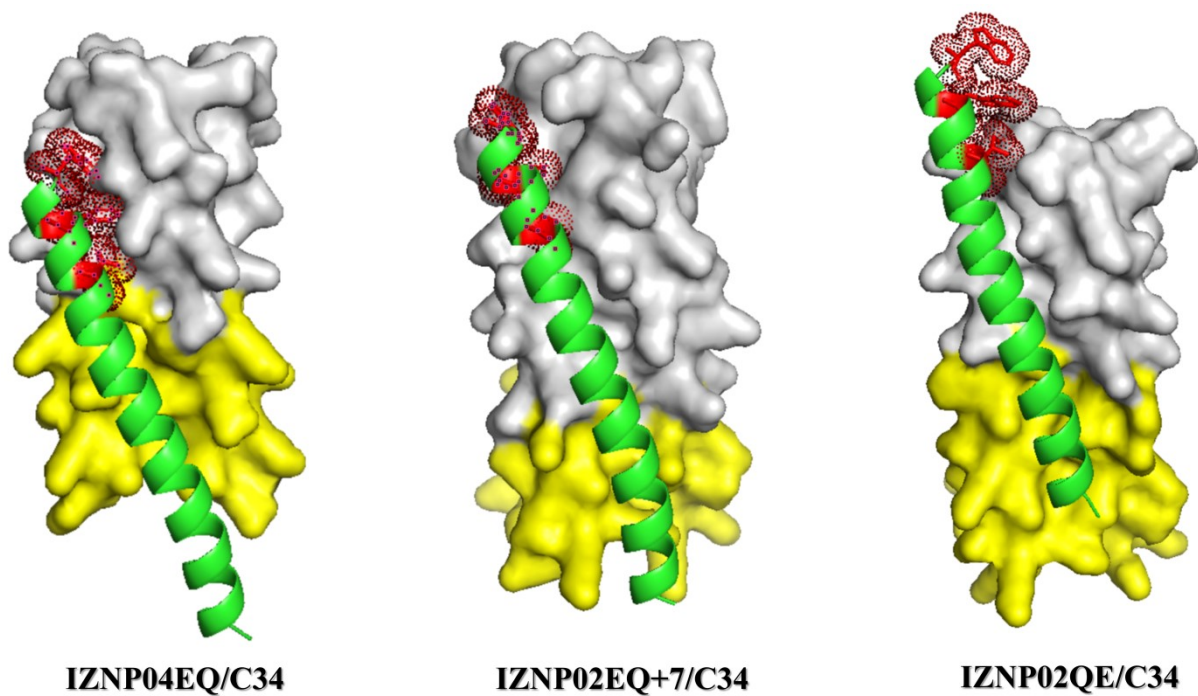


**Figure S11.** The HDOCK-based docking structure of IZNP01EK/C34, IZNP02EK/C34, IZNP03EK/C34 (Grey areas represent the pocket domains similar to NHR region, the green helix is C34 and the red amino acid residues are “WWI modif” for the binding to the pocket domains).



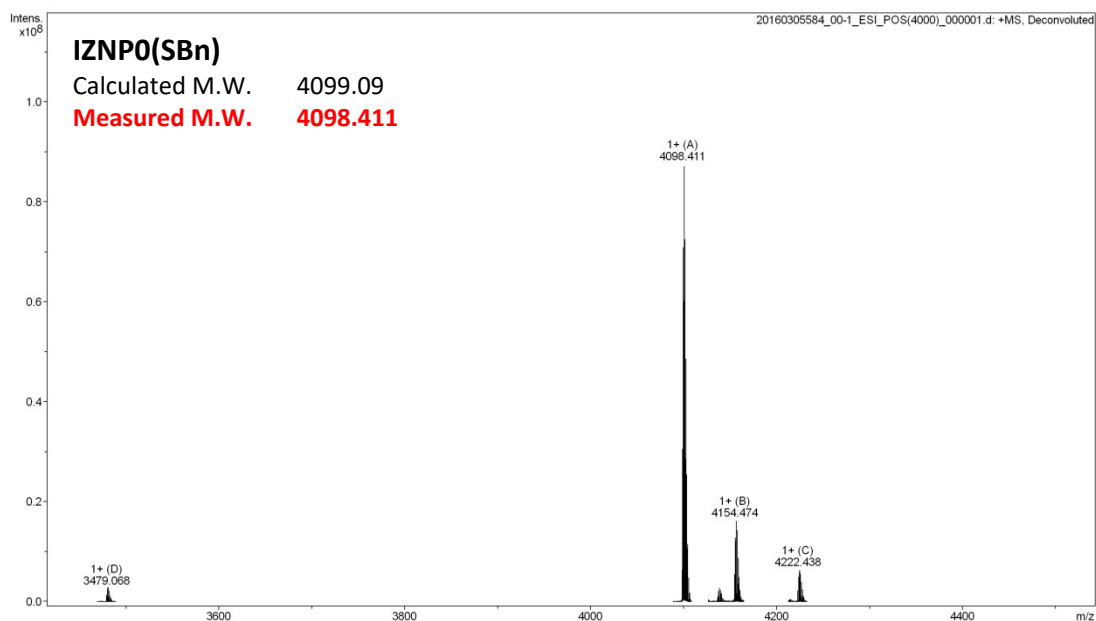
**Figure S12.** The HDOCK-based docking structure of IZNP01EQ/C34, IZNP02EQ/C34, IZNP03EQ/C34 (Grey areas represent the pocket domains similar to NHR region, the green helix is C34 and the red amino acid residues are “WWI modif” for the binding to the pocket domains).





**Figure S13.** The HDock-based docking structure of IZNP04EQ/C34, IZNP02EQ+7/C34, IZNP02QE/C34 (Grey areas represent the pocket domains similar to NHR region, the green helix is C34 and the red amino acid residues are “WWI modif” for the binding to the pocket domains).

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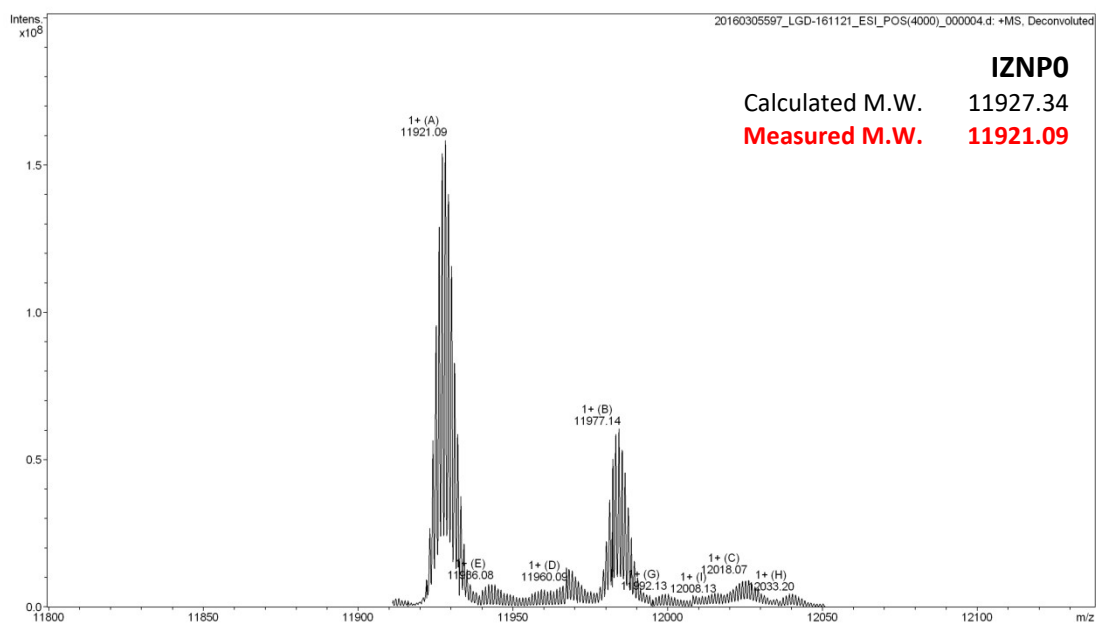
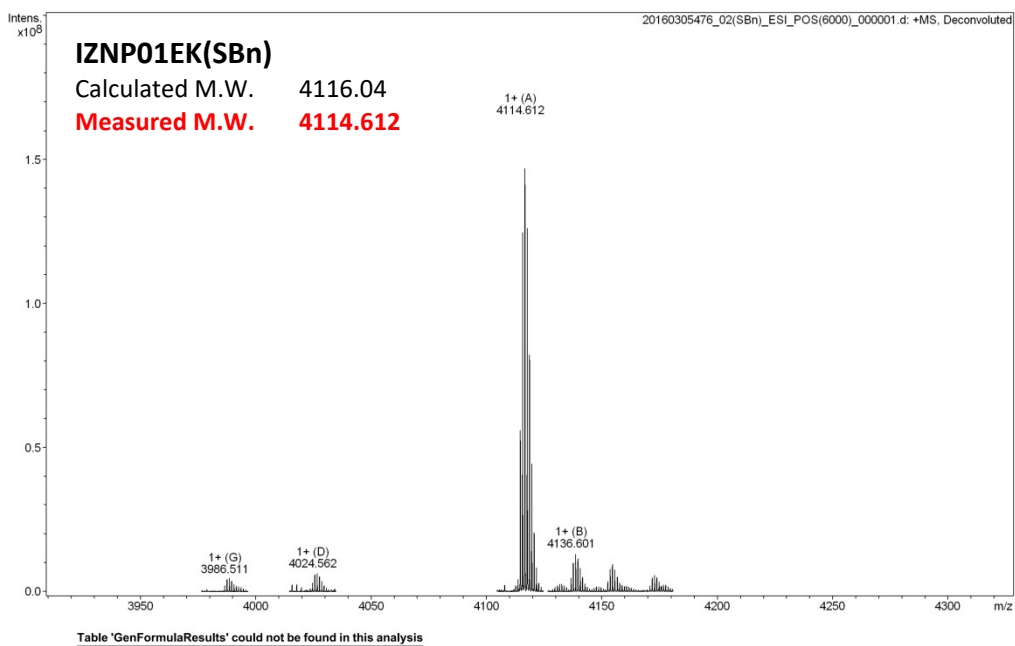


Figure S14 FT-ICR-MS spectrogram of IZNP0 thioesterified intermediate and IZNP0.

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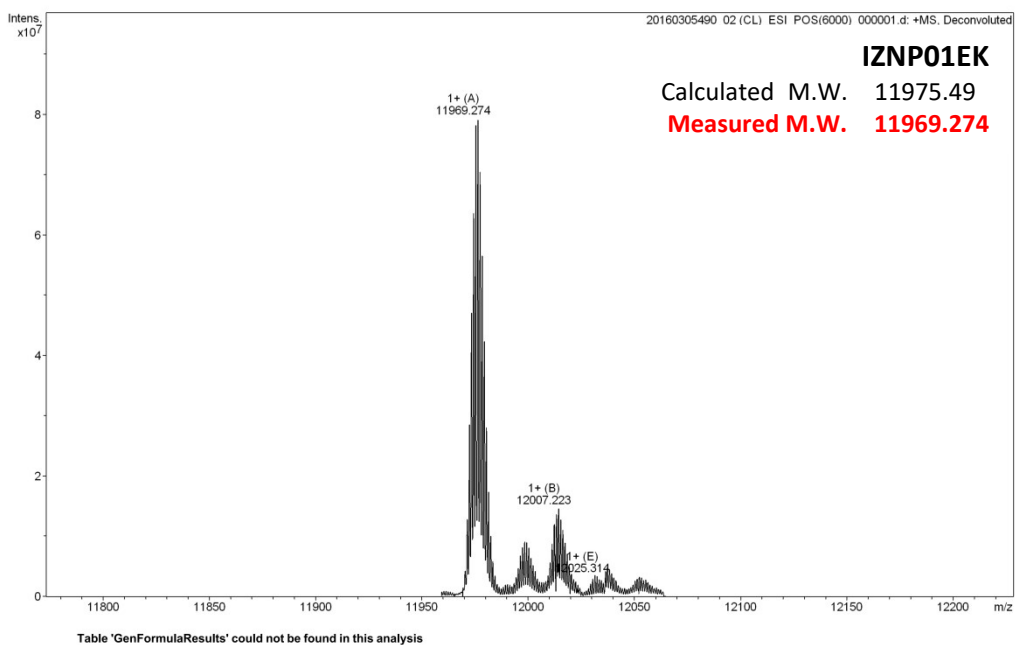
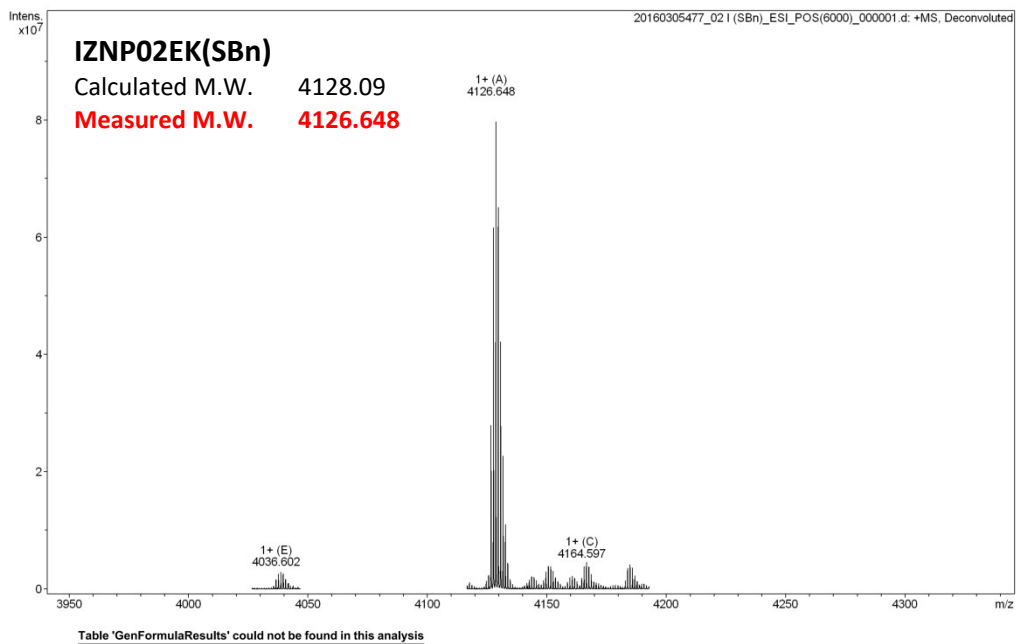


Figure S15 FT-ICR-MS spectrogram of IZNP01EK thioesterified intermediate and IZNP01EK.

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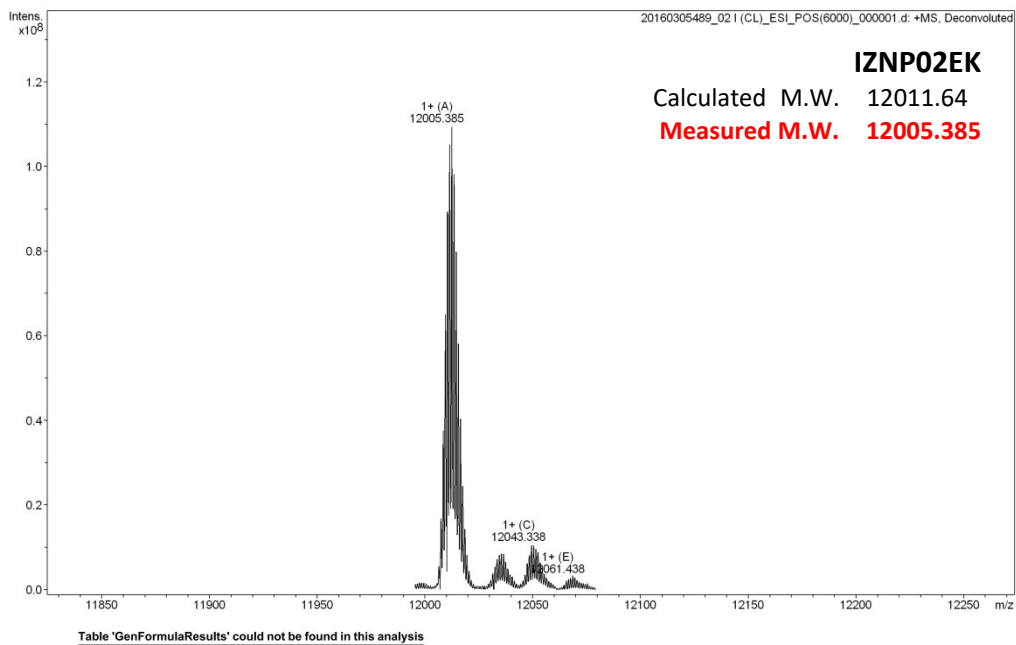
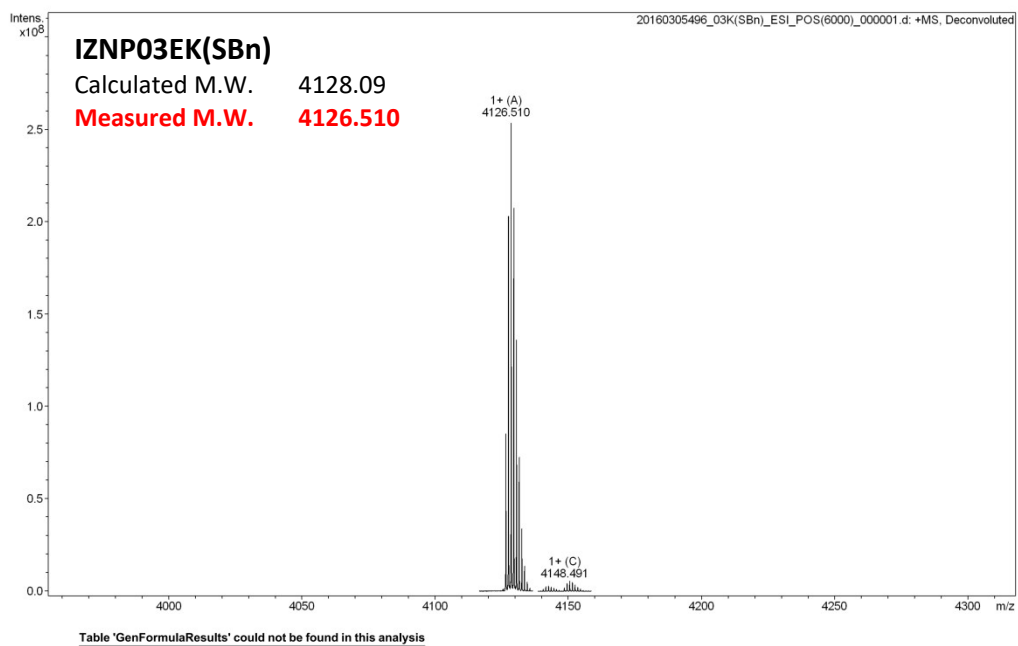
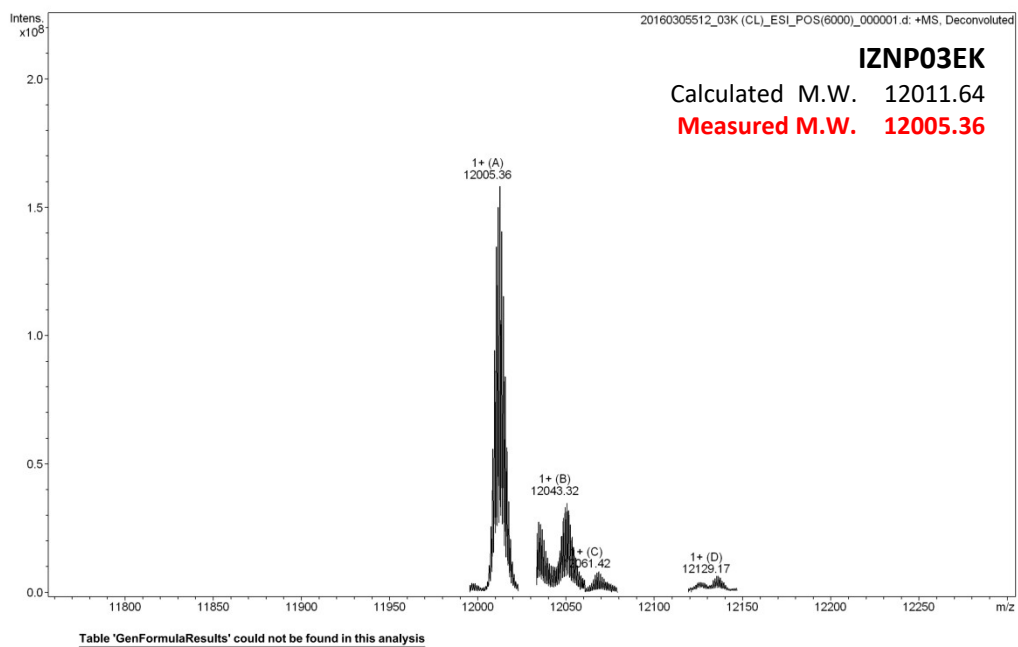


Figure S16 FT-ICR-MS spectrogram of IZNP02EK thioesterified intermediate and IZNP02EK.

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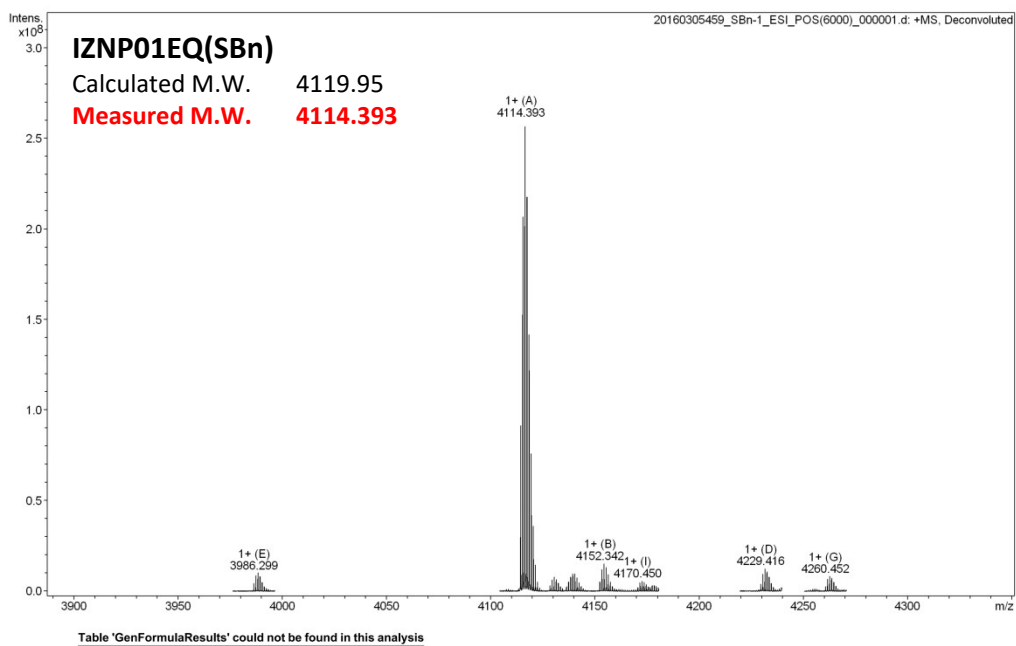


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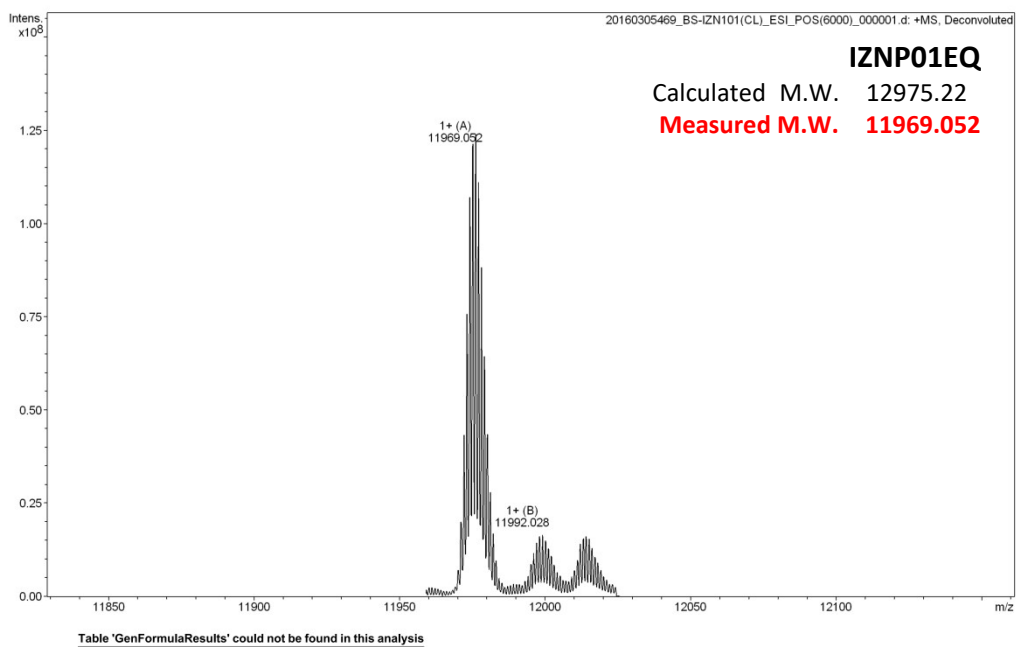


**Figure S17** FT-ICR-MS spectrogram of IZNP03EK thioesterified intermediate and IZNP03EK.

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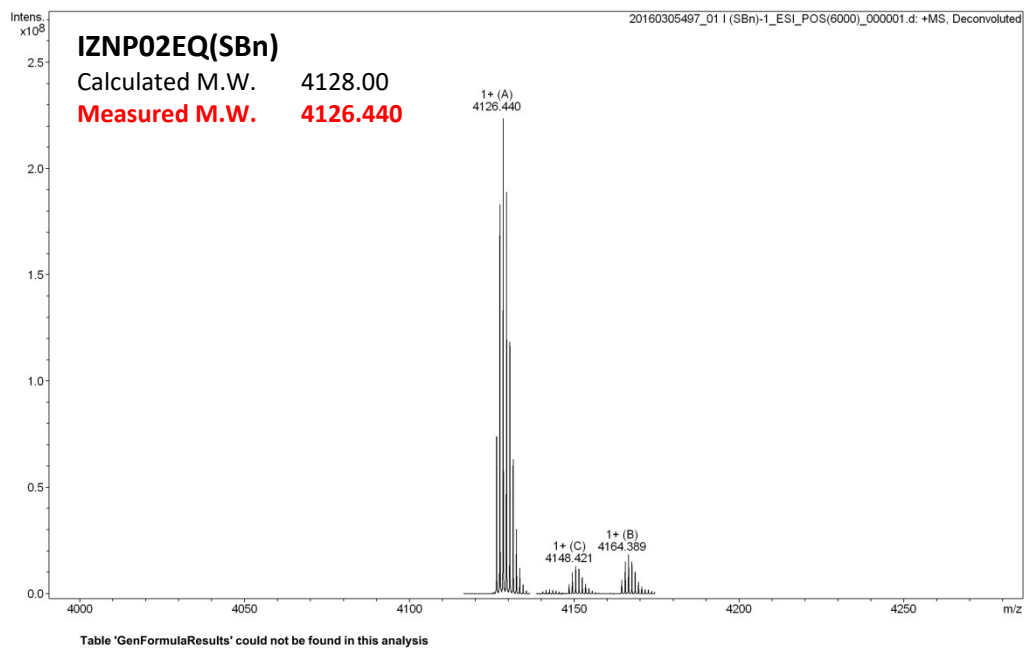


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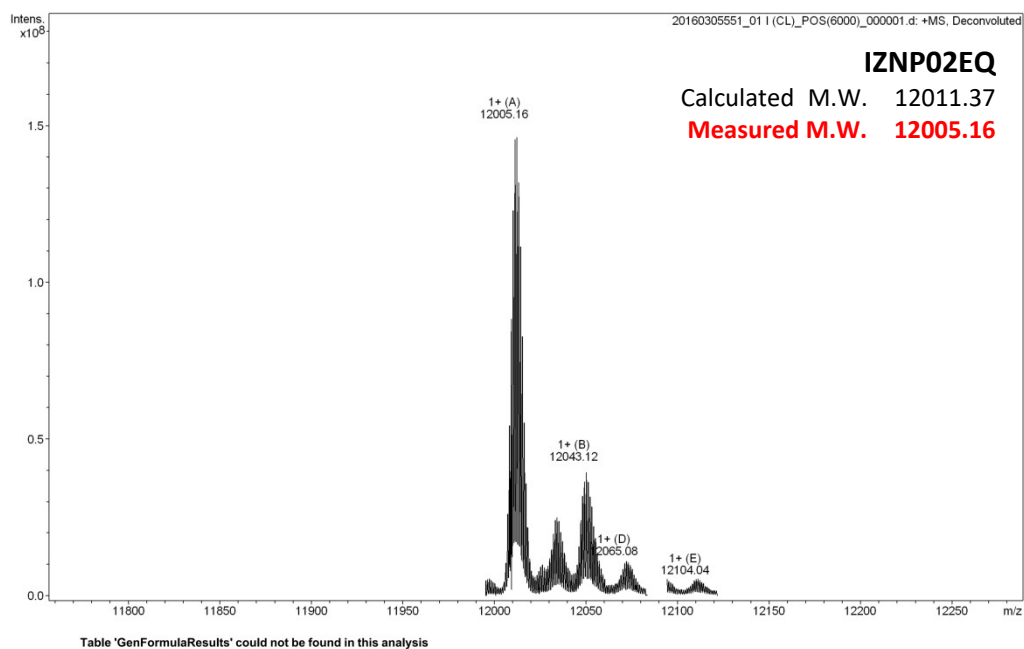


**Figure S18** FT-ICR-MS spectrogram of IZNP01EQ thioesterified intermediate and IZNP01EQ.

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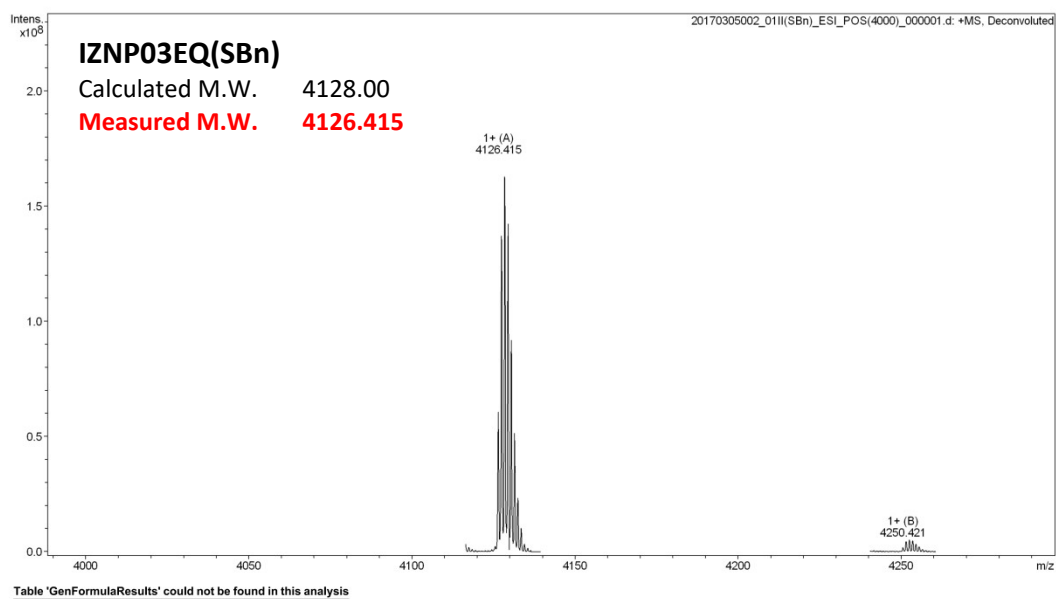


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**Figure S19** FT-ICR-MS spectrogram of IZNP02EQ thioesterified intermediate and IZNP02EQ.

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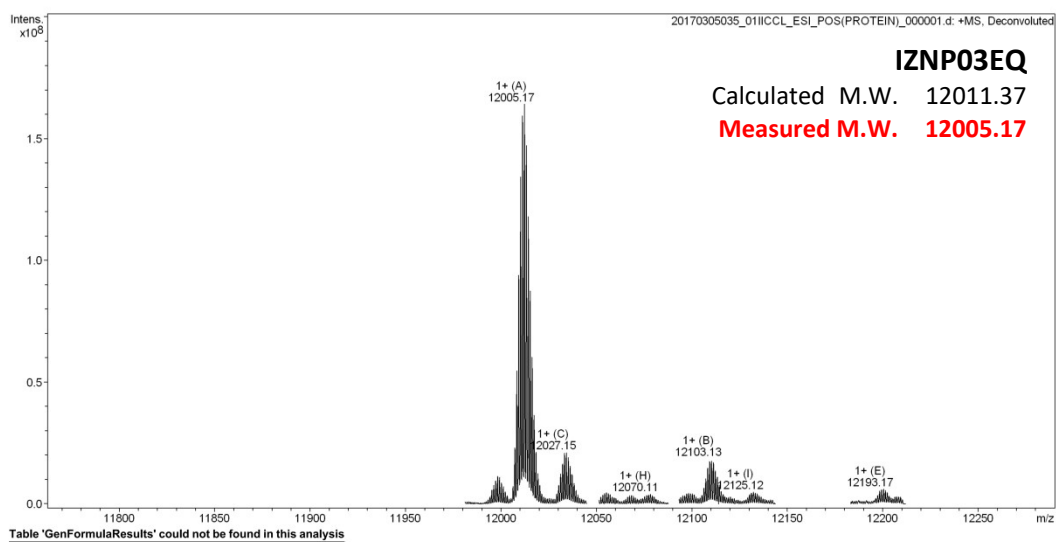


Figure S20 FT-ICR-MS spectrogram of IZNP03EQ thioesterified intermediate and IZNP03EQ.



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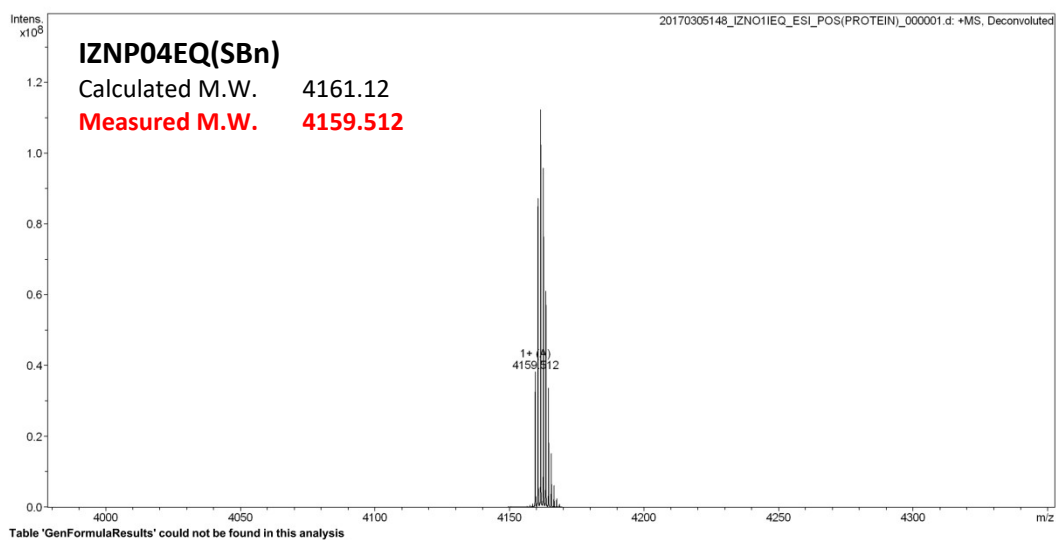


Figure S21 FT-ICR-MS spectrogram of IZNP04EQ thioesterified intermediate.

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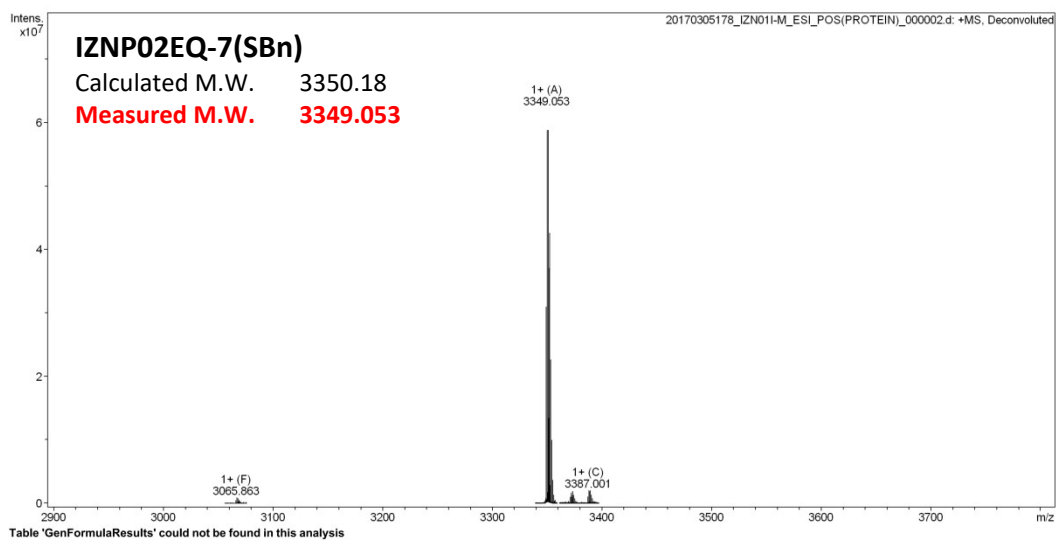
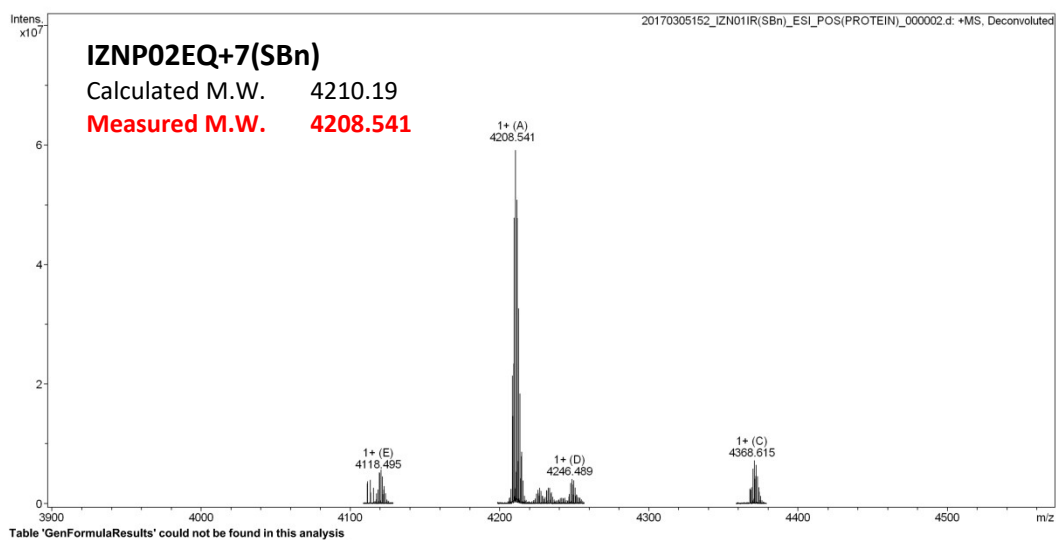


Figure S22 FT-ICR-MS spectrogram of IZNP02EQ-7 thioesterified intermediate.

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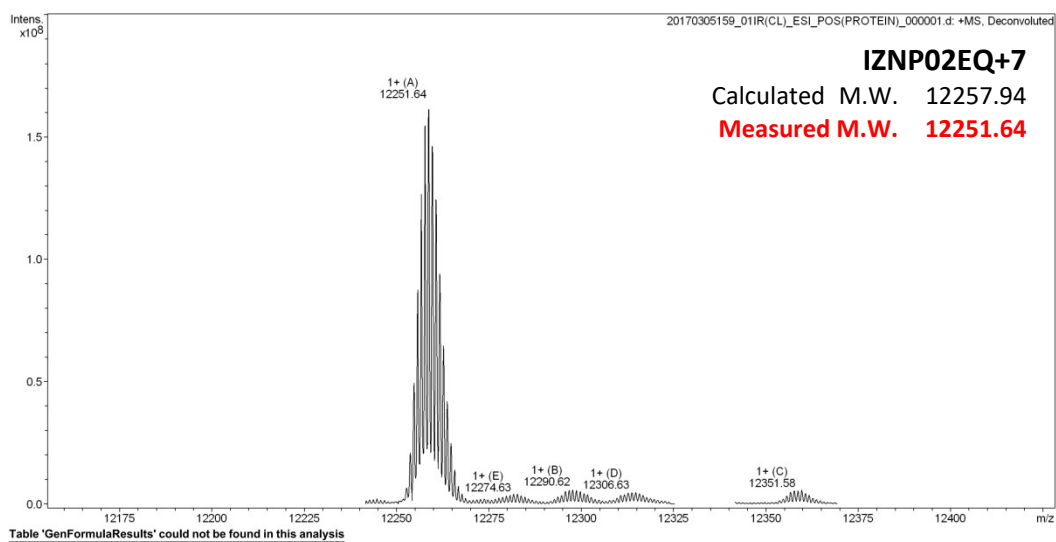
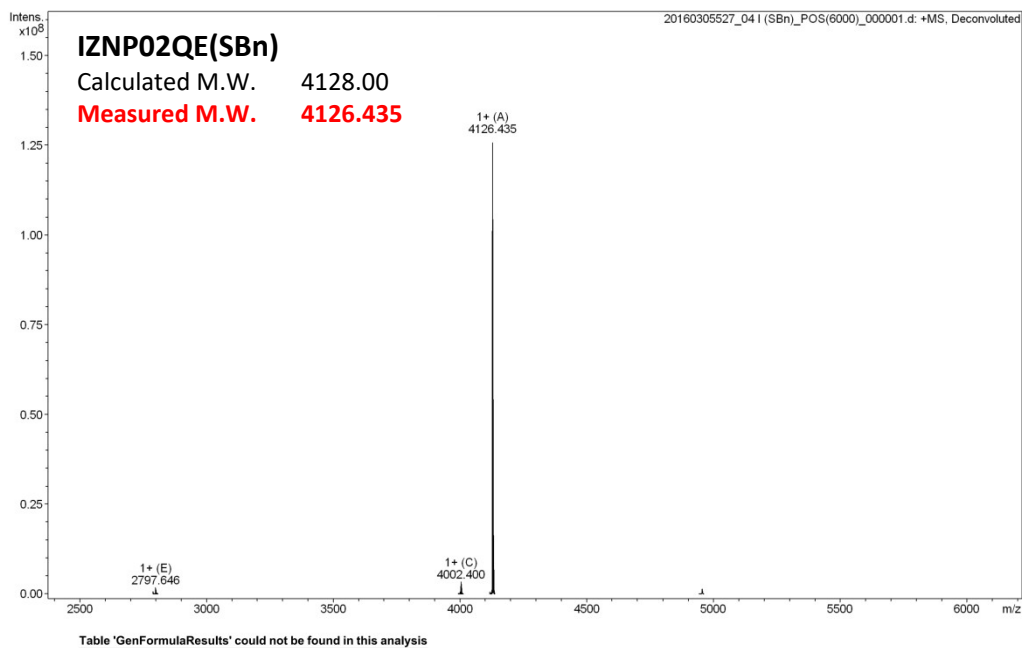


Figure S23 FT-ICR-MS spectrogram of IZNP02EQ+7 thioesterified intermediate and IZNP02EQ+7.

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### Mass Spectrum Molecular Formula Report

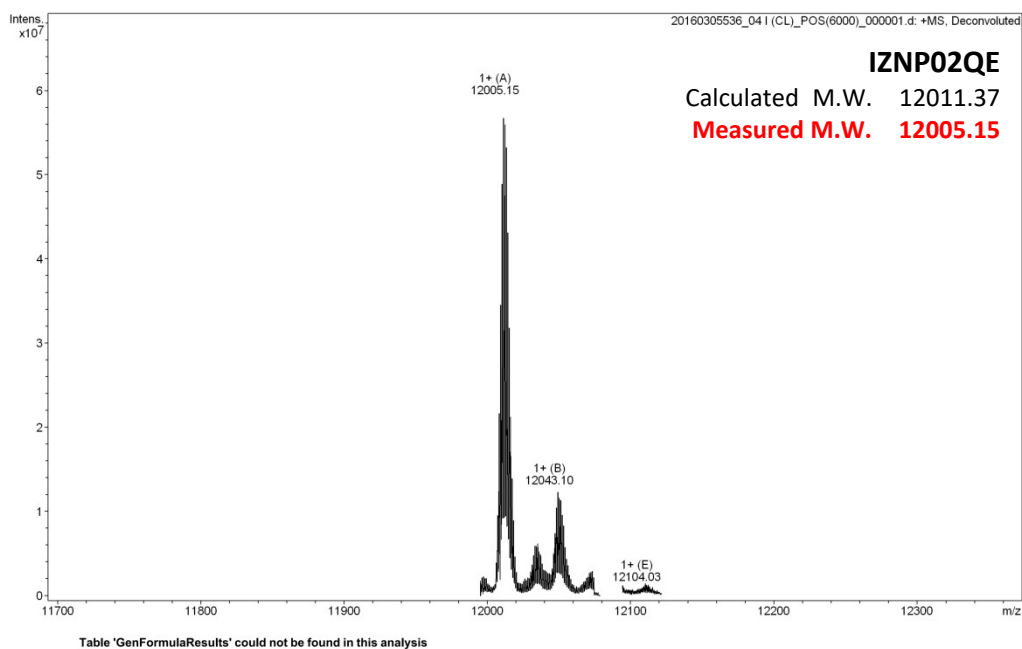


Figure S24 FT-ICR-MS spectrogram of IZNP02EQ+7 thioesterified intermediate and IZNP02EQ+7.