# APPENDIX

## A. Influencing Factors

We comprehensively show the results of influencing factors in Figure 3 and Figure 4 on Seven-species dataset and HC-PT dataset, respectively. The detailed analysis for these results can be found in the main texts.

## B. Corrected Results for InstaNovo

In the main body of the text, we utilized the original open-source code of InstaNovo for training and testing, only to find that the results were significantly lower than expected. Therefore, after the deadline of the main text, we re-implemented InstaNovo and have since corrected its results. We will also incorporate these new results into the main body of the text in the future.

Table 6: Corrected results for InstaNovo.

| Metric | Seven-species | Nine-species | HC-PT |
|---|---|---|---|
| AA. Prec. | 0.192 | 0.420 | 0.289 |
| AA. Recall | 0.176 | 0.395 | 0.285 |
| Pep. Prec. | 0.031 | 0.164 | 0.057 |
| Pep. AUC | 0.009 | 0.123 | 0.034 |
| PTM Recall | 0.115 | 0.294 | 0.261 |
| PTM Prec. | 0.126 | 0.443 | 0.350 |
| Confidence score | 0.665 | 0.782 | 0.652 |
| Training Time | 0.90 | 0.86 | 0.79 |
| Inference Time | 0.46 | 0.39 | 0.37 |
| Trainable Params | 92.3 | 92.3 | 92.3 |

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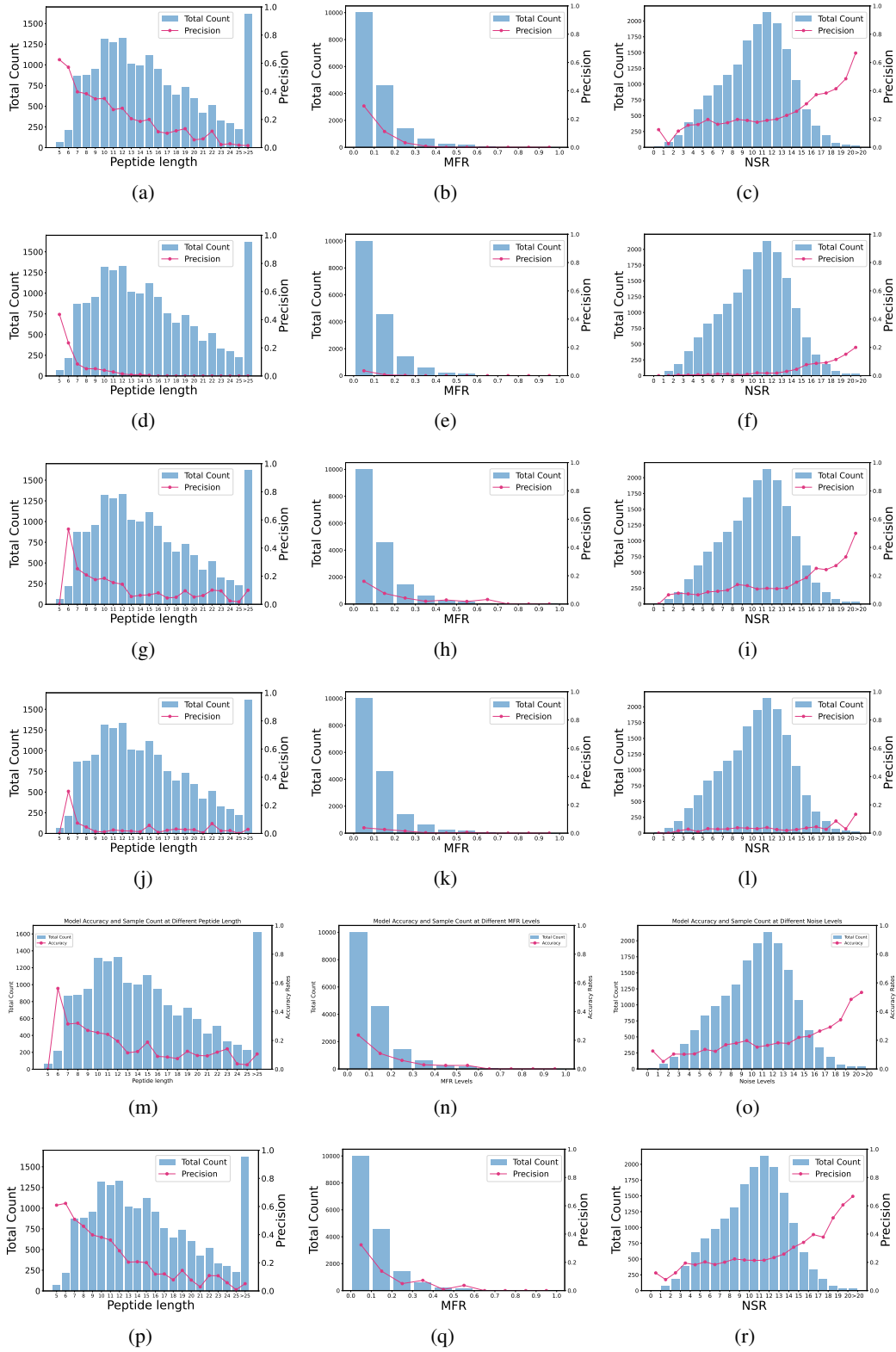
Figure 3: Peptide-level precision curves of the benchmarking models under the influence of three factors on Seven-species dataset. The first row to the sixth row correspond to the models DeepNovo, PointNovo, CasaNovo, InstaNovo, AdaNovo, $\pi$-HelixNovo, and the first column to the third column correspond to the three influencing factors Peptide length, missing fragmentation ratio (MFR) and noise peaks (NSR).

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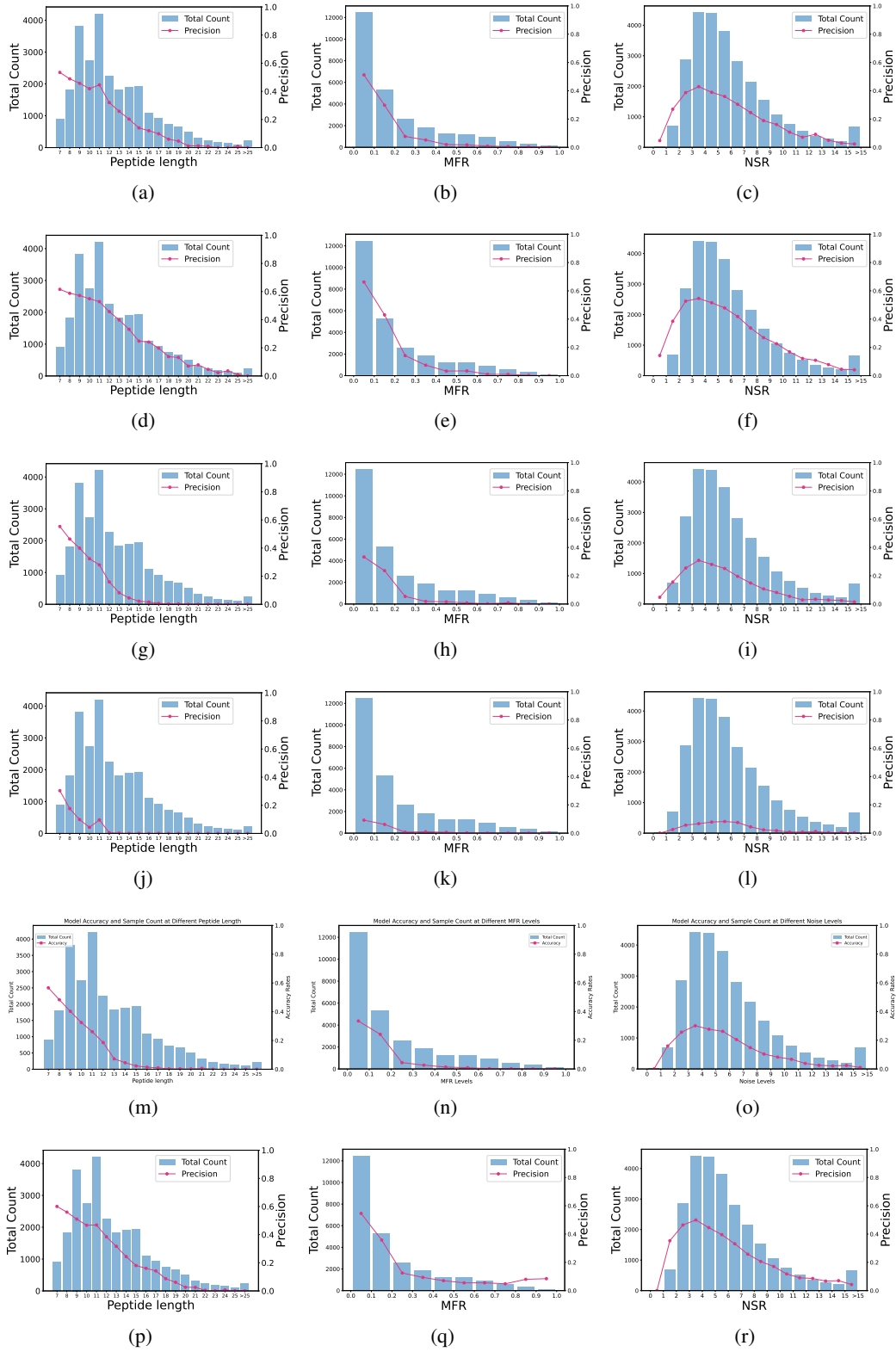
Figure 4: Peptide-level precision curves of the benchmarking models under the influence of three factors on HC-PT dataset. The first row to the sixth row correspond to the models DeepNovo, PointNovo, CasaNovo, InstaNovo, AdaNovo, $\pi$-HelixNovo, and the first column to the third column correspond to the three influencing factors Peptide length, missing fragmentation ratio (MFR) and noise peaks (NSR).

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