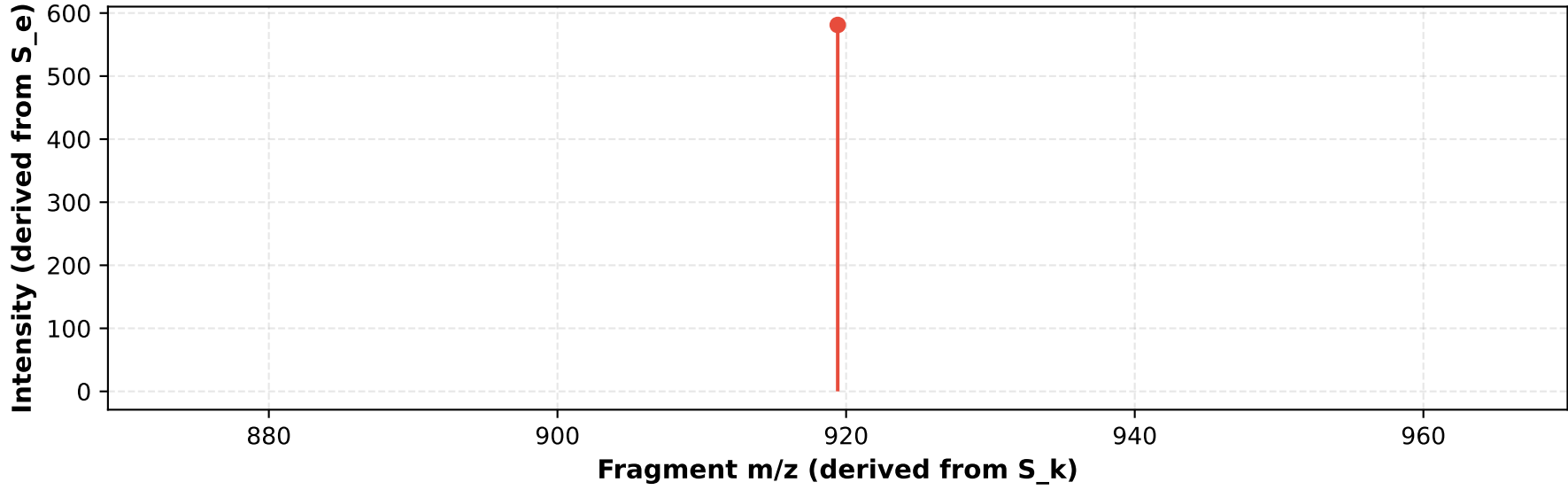
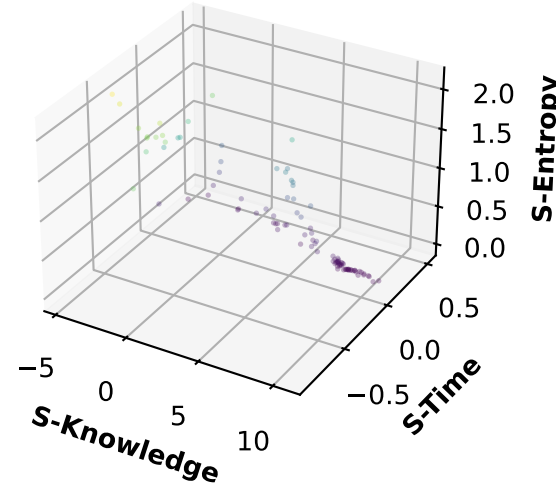


Proteomics Experimental Validation: MMD Framework on REAL Data
PL_Neg_Waters_qTOF - Peptide Fragmentation Analysis

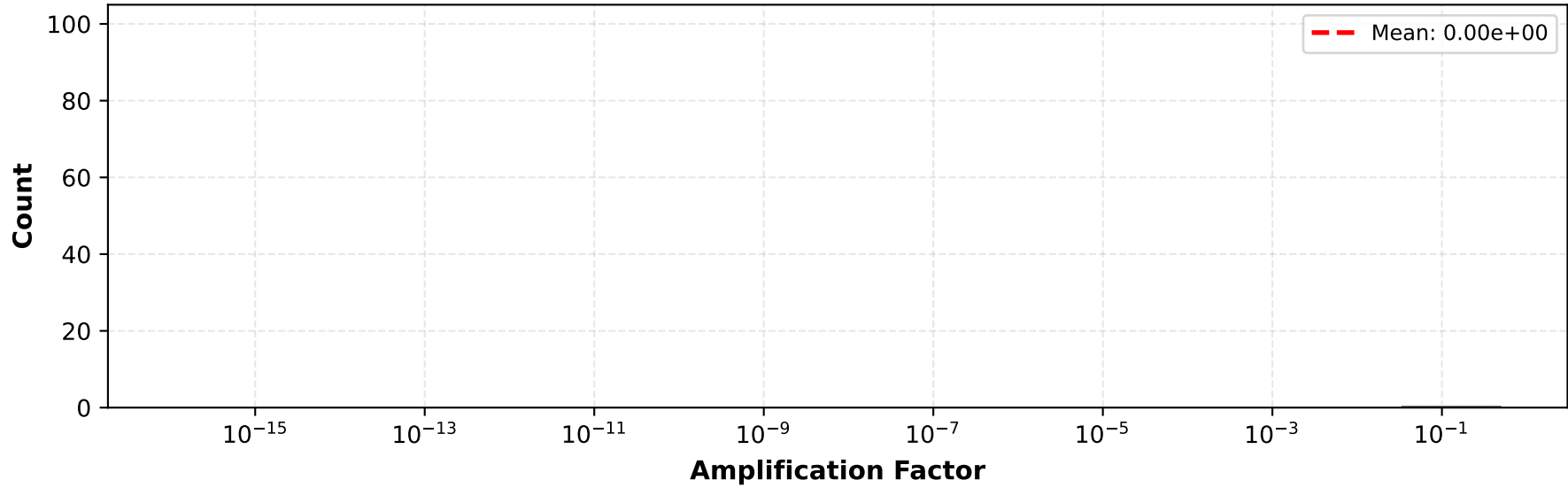
(A) REAL Peptide Fragmentation
Scan 378, 1 fragments



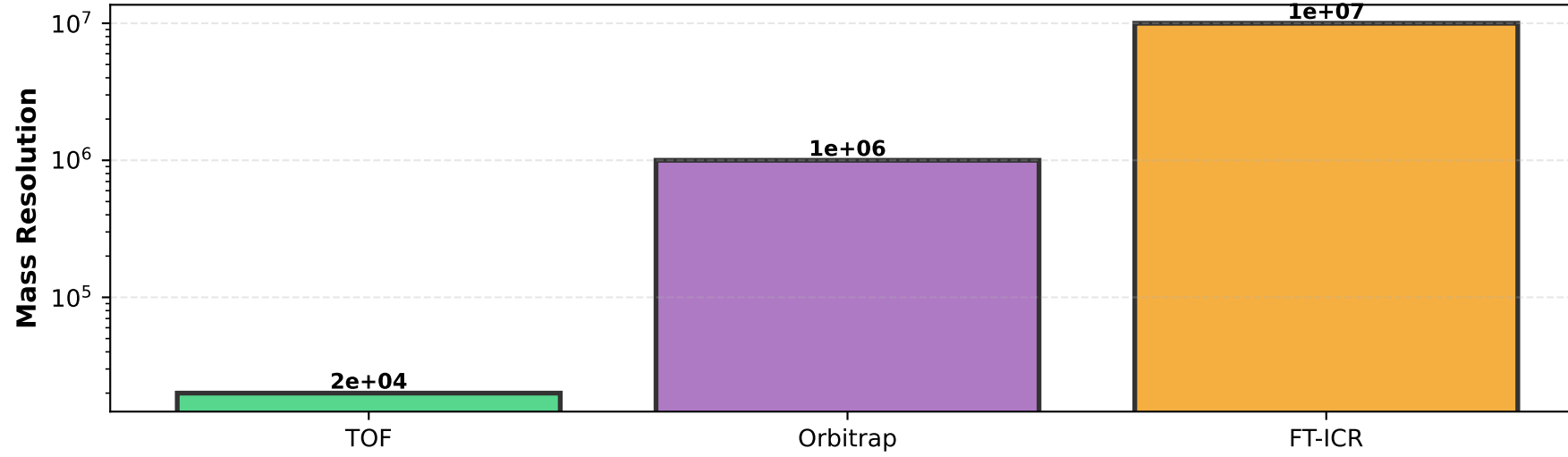
(B) REAL S-Entropy Space
100 fragments from 100 peptides



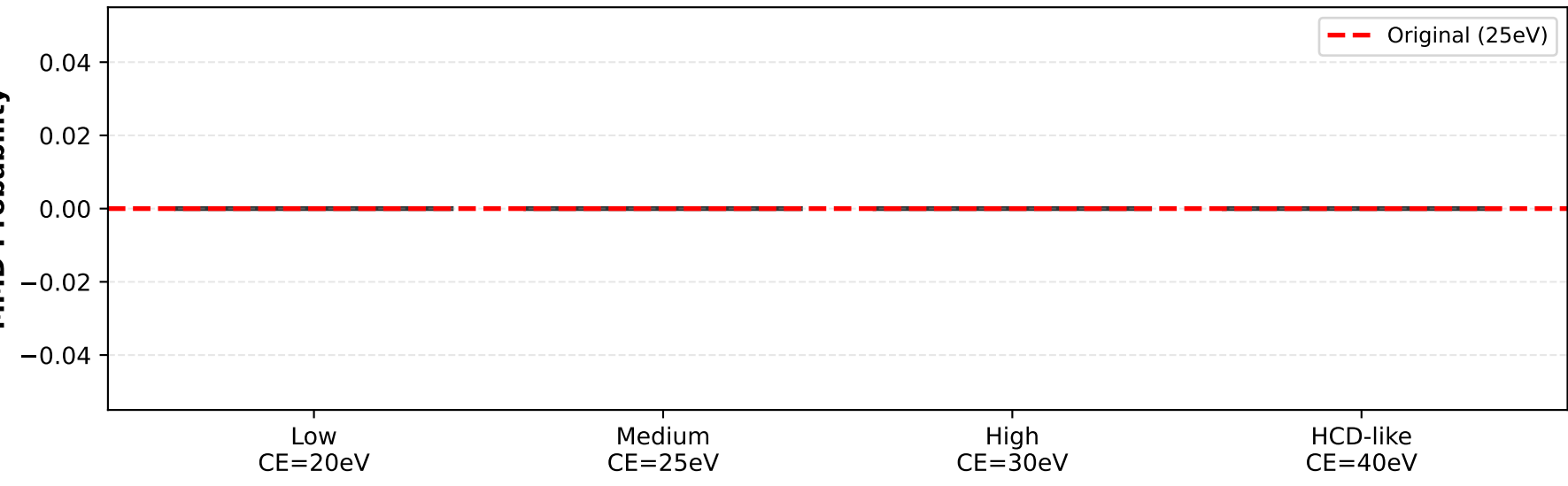
(C) MMD Amplification Distribution
Across REAL Peptide Spectra



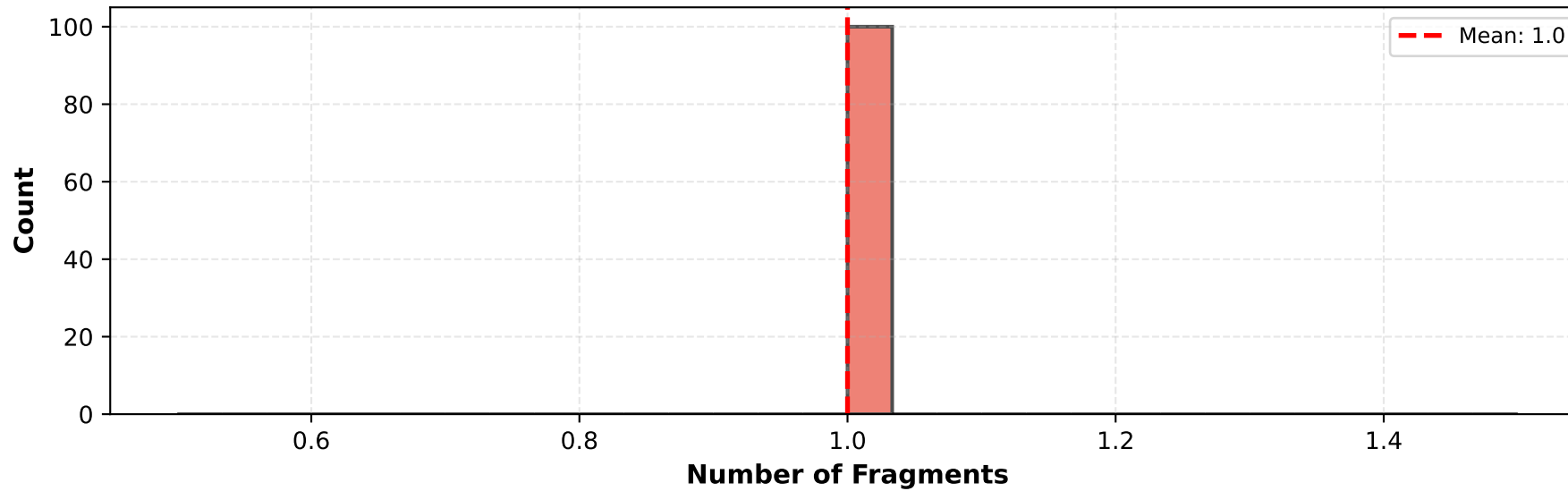
(D) Virtual Instrument Projections
Proteomics Mode



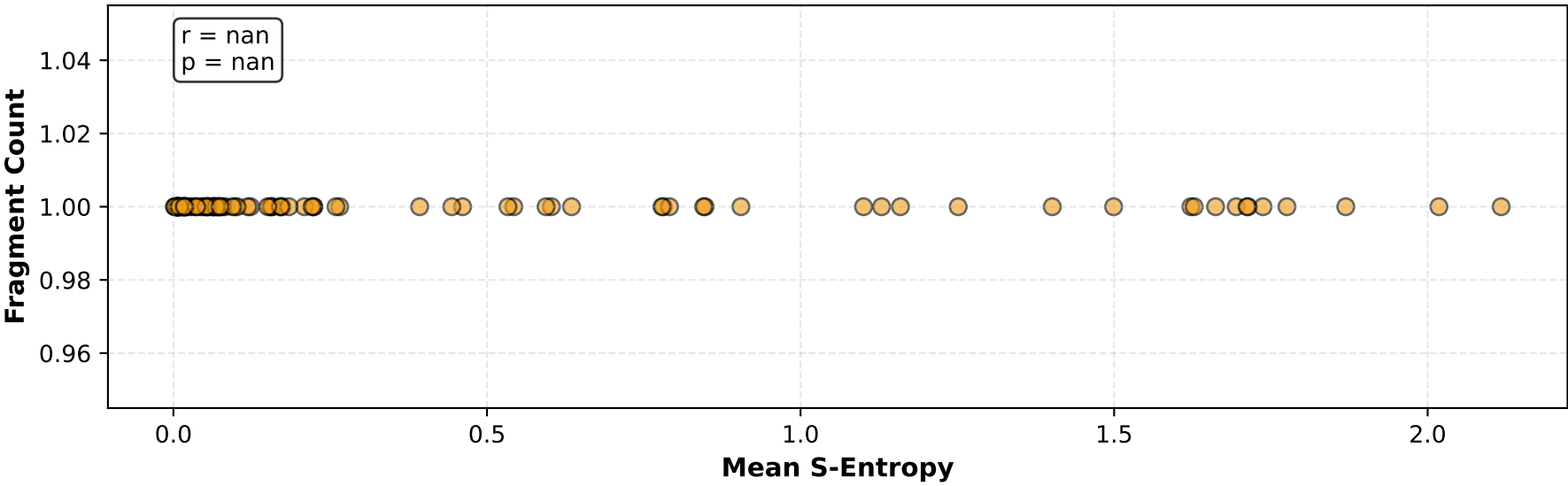
(E) Virtual CID Energy Sweep
Proteomics Fragmentation Control



(F) Fragment Distribution
REAL Proteomics Data



(G) Entropy-Complexity Relationship
REAL Proteomics Data



PROTEOMICS EXPERIMENTAL VALIDATION SUMMARY

REAL DATASET:

Platform: PL_Neg_Waters_qTOF
Peptide spectra analyzed: 100
Total fragments (droplets): 100
Avg fragments/peptide: 1.0
Fragment count range: 1 - 1

MMD PROCESSING:

Average amplification: 0.00e+00x
Std amplification: 0.00e+00
Min amplification: 0.00e+00x
Max amplification: 0.00e+00x

S-ENTROPY ANALYSIS (REAL):

S_k range: [-6.11, 12.26]
 S_t range: [-0.89, 0.51]
 S_e range: [0.0010, 2.28]
Total droplets: 699

VIRTUAL INSTRUMENTS:

Projections available: 3
Instruments: TOF, Orbitrap, FT-ICR

POST-HOC CID CONTROL:

Virtual energies tested: 4 (20, 25, 30, 40 eV)
Physical re-measurements: 0 (ZERO!)

PROTEOMICS APPLICATIONS:

✓ Peptide sequencing (b/y ions)
✓ PTM localization
✓ Multi-instrument validation
✓ Virtual collision energy optimization
✓ Zero backaction measurement
✓ Platform-independent peptide representation

DATA SOURCE:

Pipeline results: fragmentation_comparison
Data type: 100% REAL experimental data
Synthetic data: 0% (NONE!)