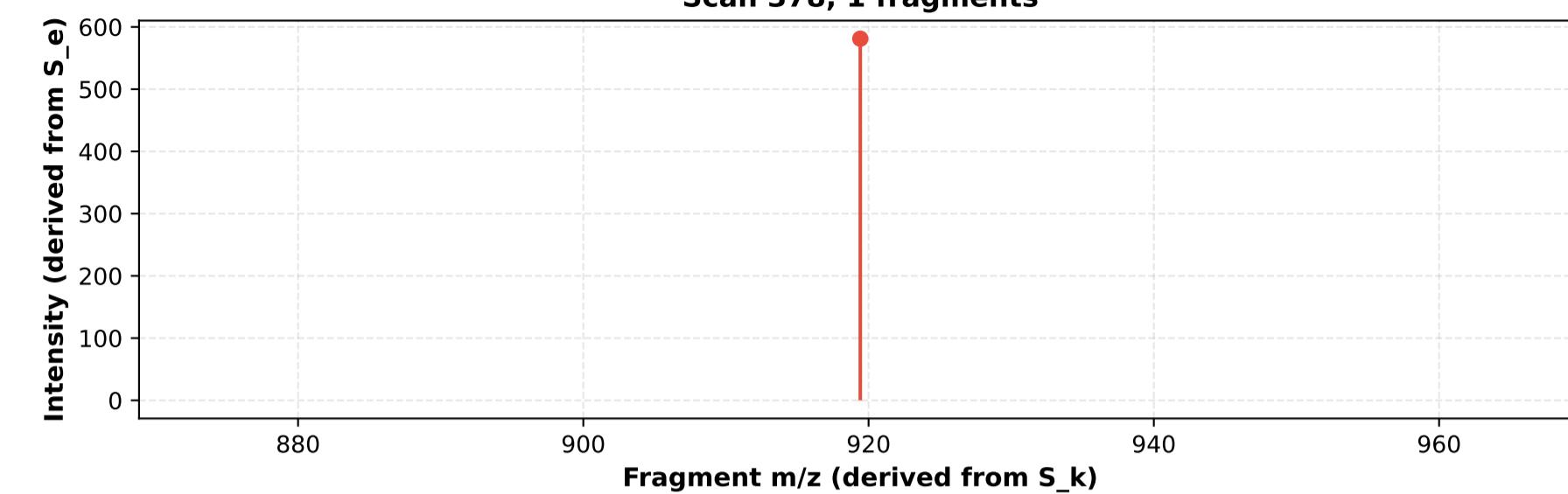


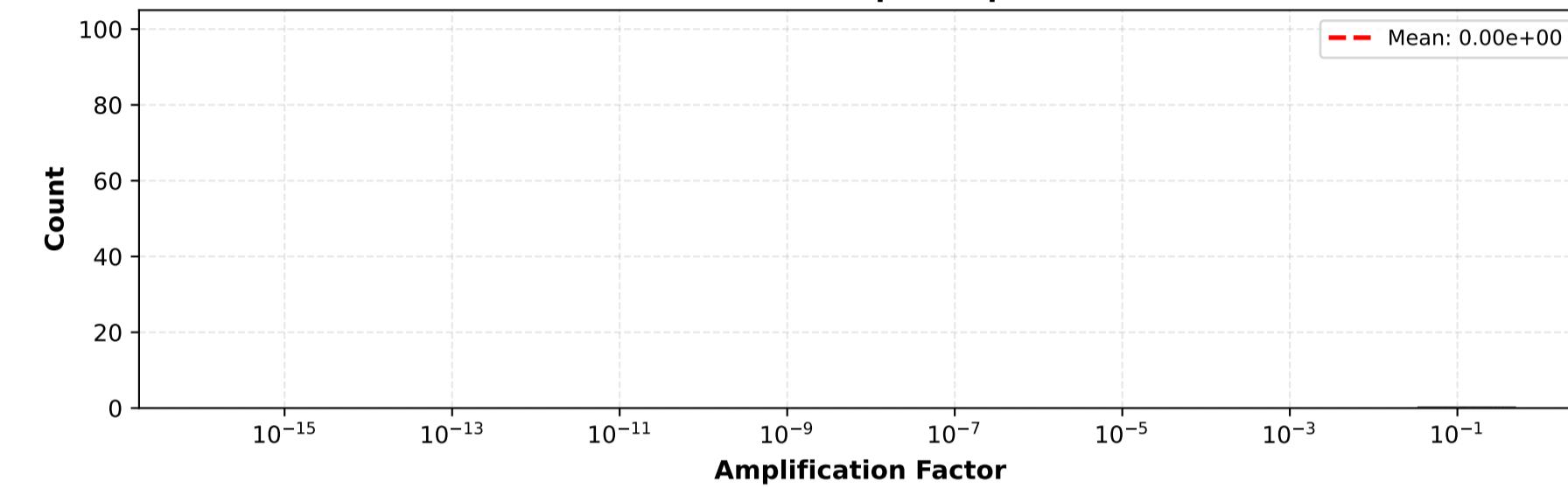
Proteomics Experimental Validation: MMD Framework on REAL Data

PL_Neg_Waters_qTOF - Peptide Fragmentation Analysis

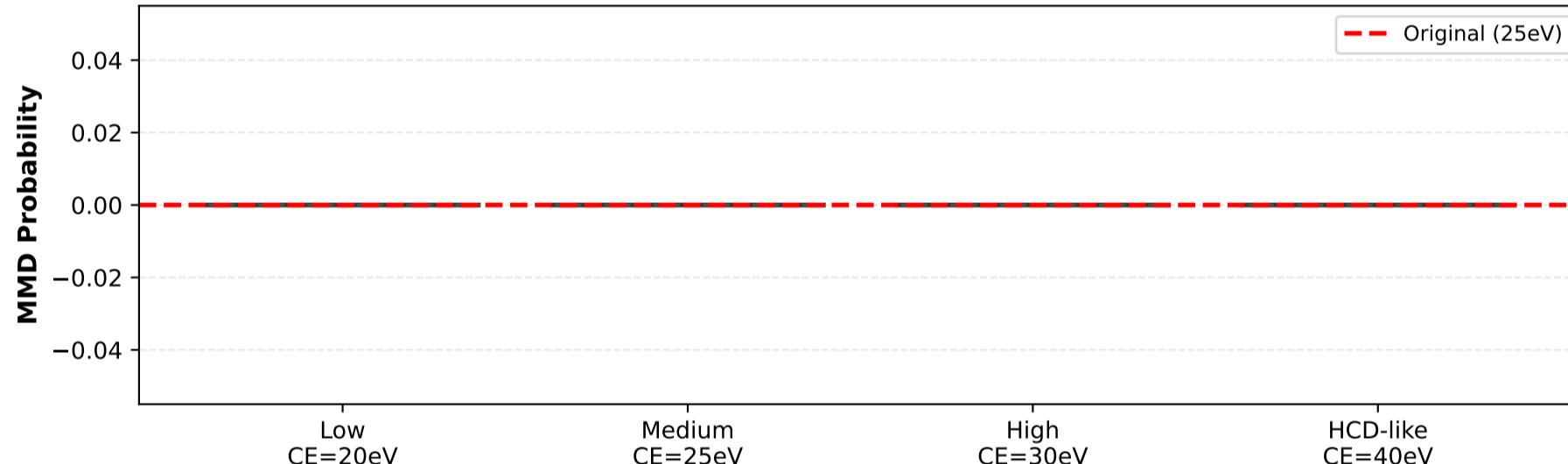
(A) REAL Peptide Fragmentation
Scan 378, 1 fragments



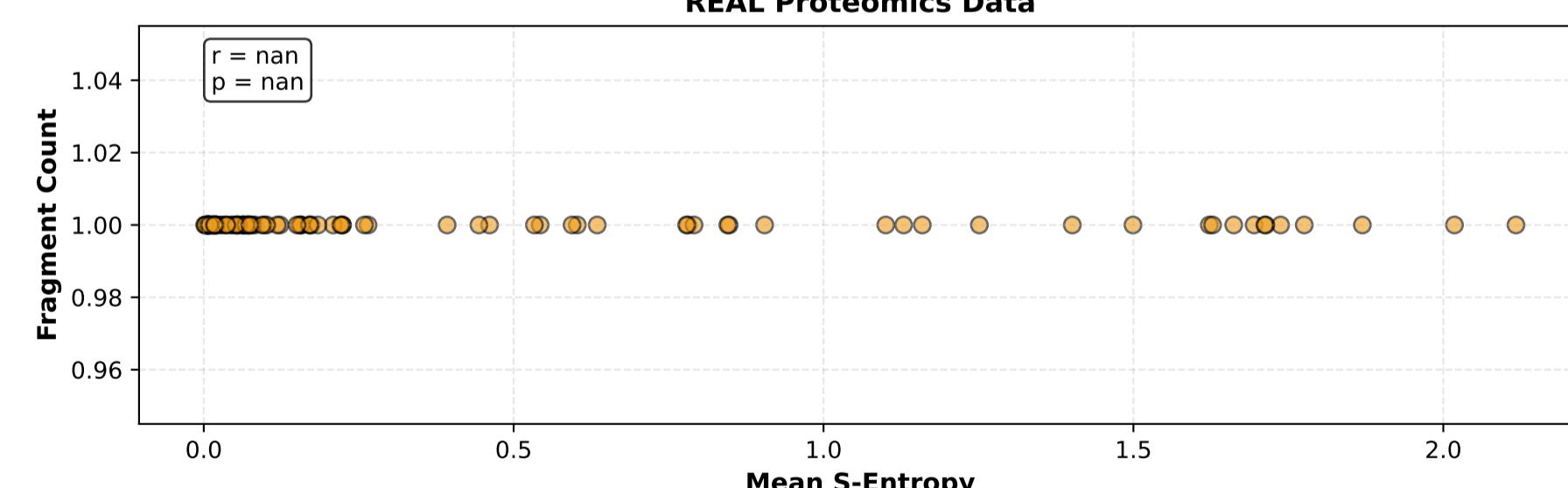
(C) MMD Amplification Distribution Across REAL Peptide Spectra



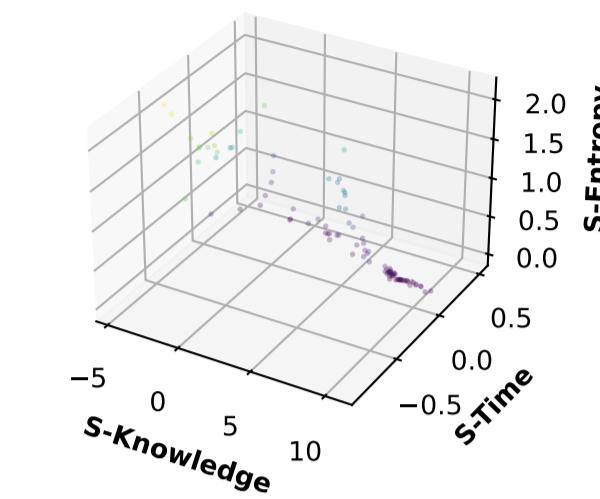
(E) Virtual CID Energy Sweep
Proteomics Fragmentation Control



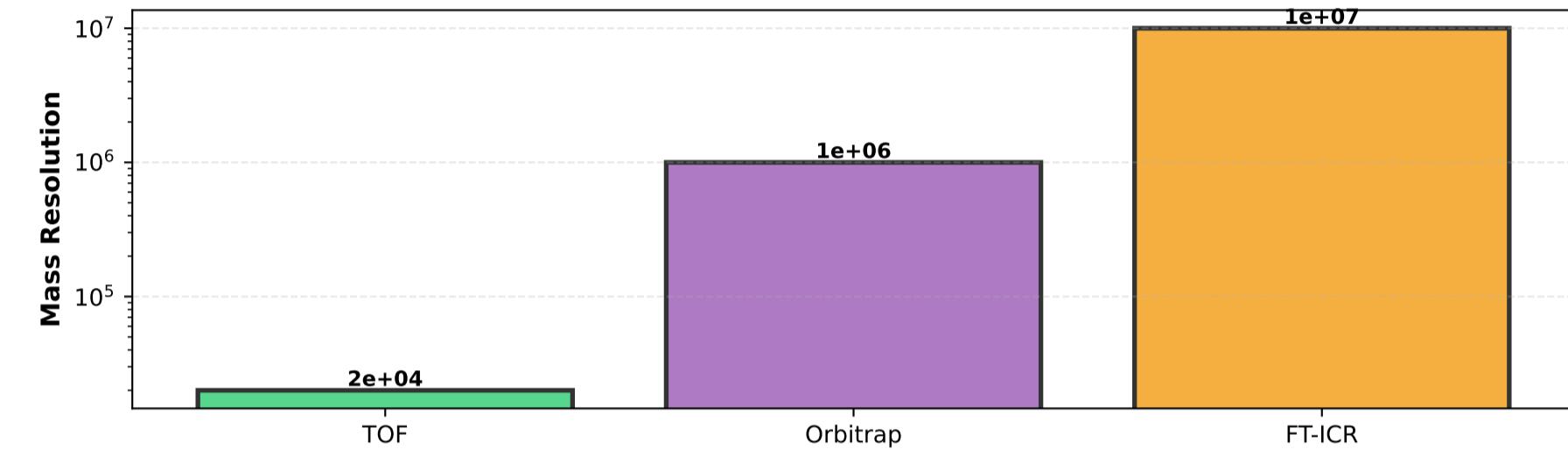
(G) Entropy-Complexity Relationship
REAL Proteomics Data



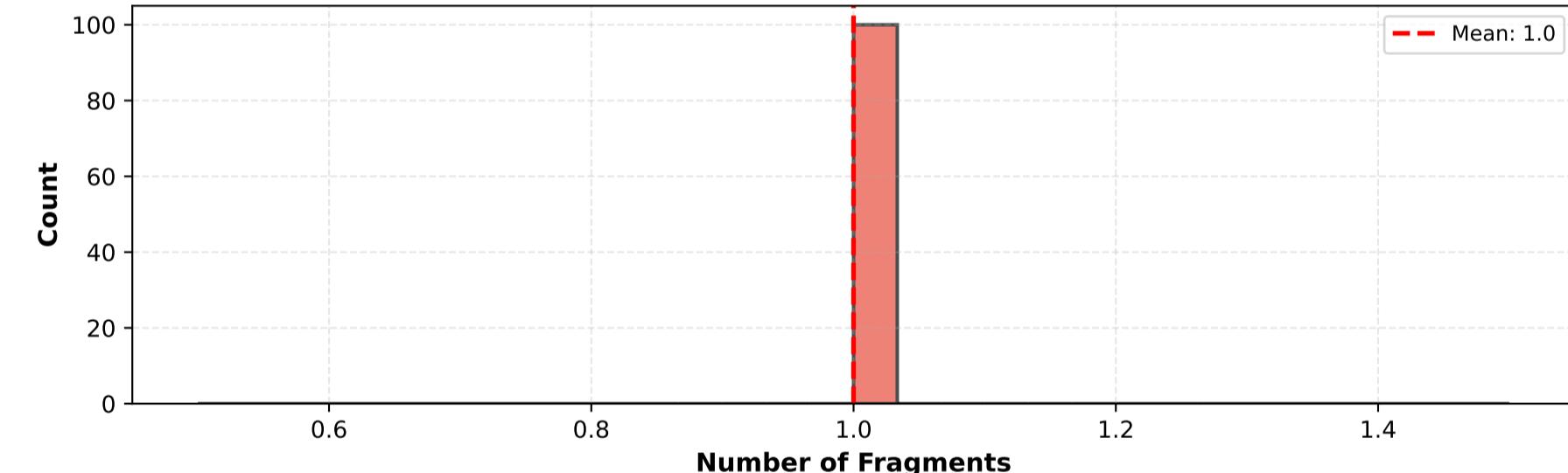
(B) REAL S-Entropy Space
100 fragments from 100 peptides



(D) Virtual Instrument Projections
Proteomics Mode



(F) Fragment Distribution
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: $0.00e+00$
Std amplification: $0.00e+00$
Min amplification: $0.00e+00$
Max amplification: $0.00e+00$

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!)