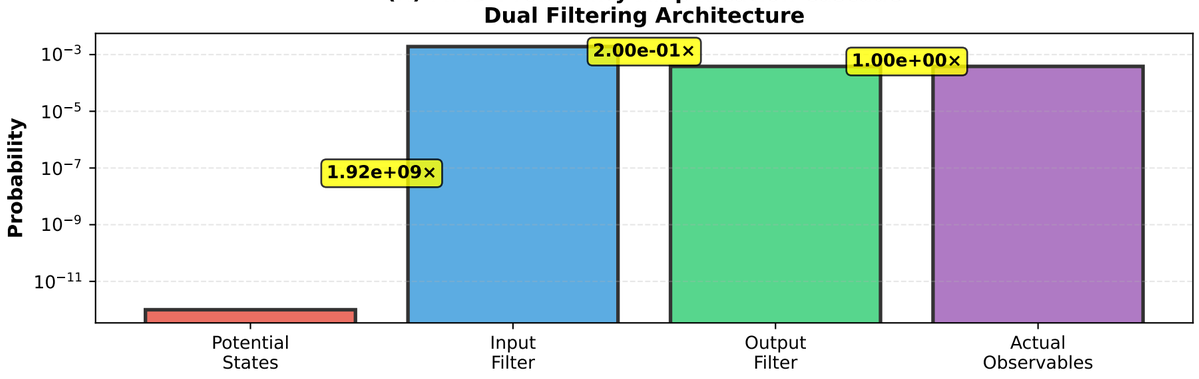
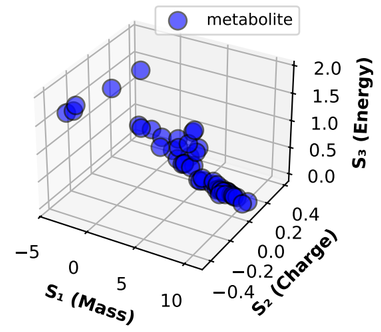
Molecular Maxwell Demon Mass Spectrometry Framework - REAL DATA
Information Catalysis for Post-Hoc Virtual Measurements

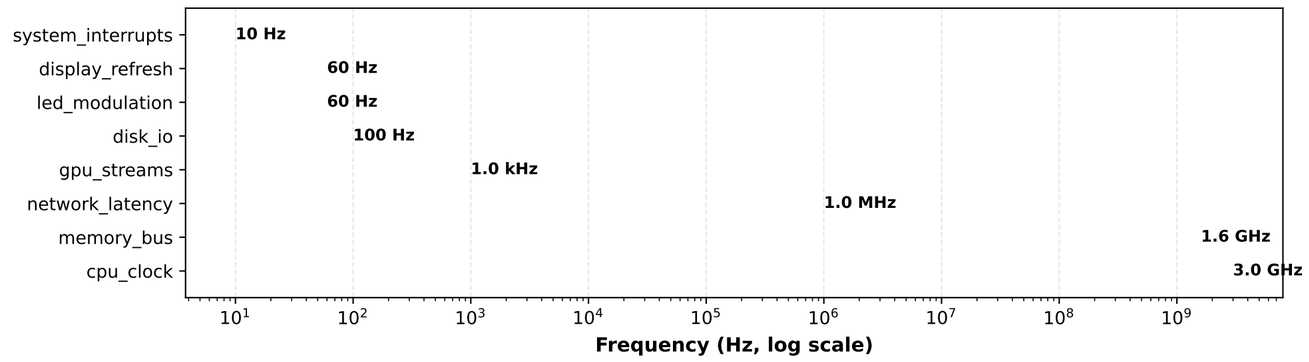
(A) MMD Probability Amplification Cascade
Dual Filtering Architecture



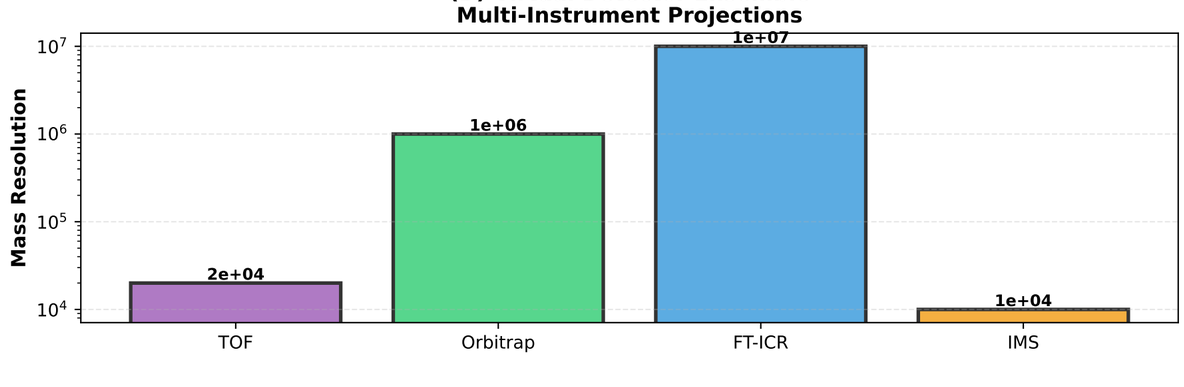
(B) S-Entropy Coordinate Space
14D → 3D Projection



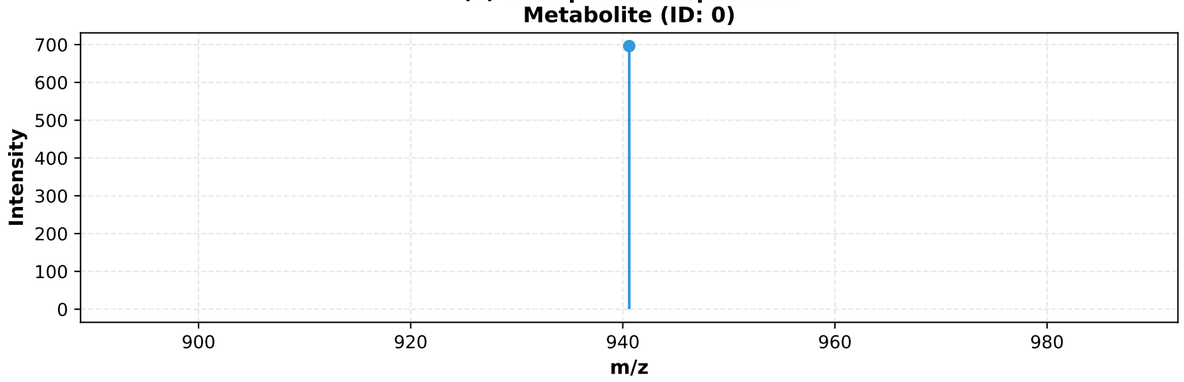
(C) Hardware Oscillation Hierarchy
8-Scale Phase-Lock Architecture



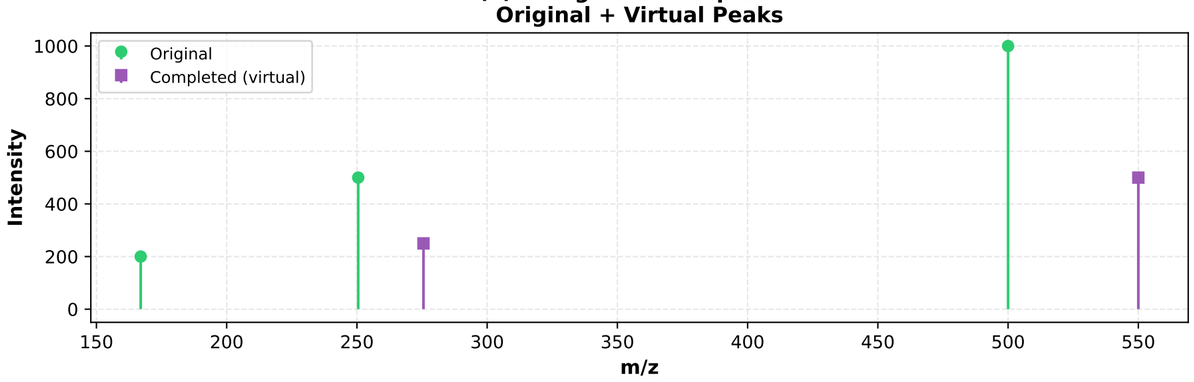
(D) Virtual Detector Ensemble
Multi-Instrument Projections



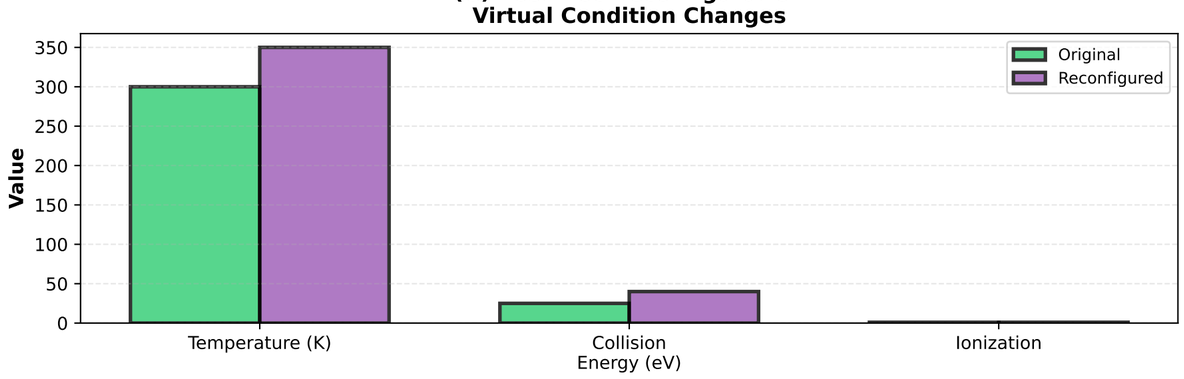
(E) Example Mass Spectrum
Metabolite (ID: 0)



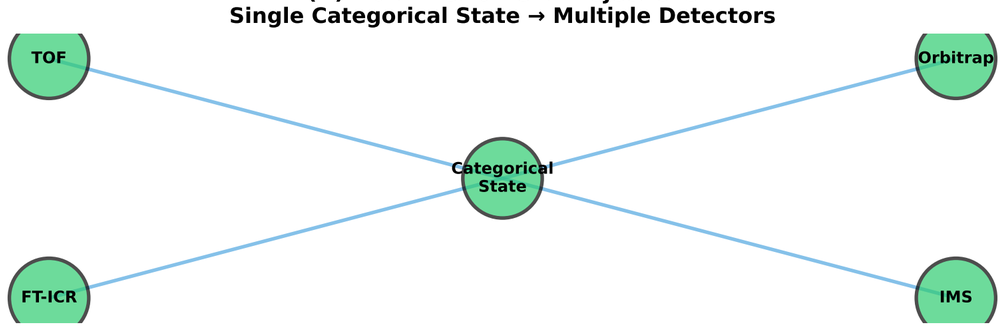
(F) Categorical Completion
Original + Virtual Peaks



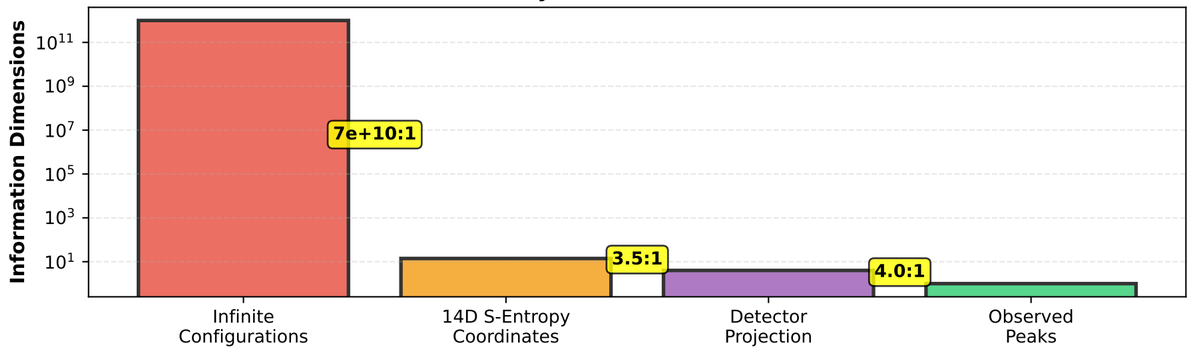
(G) Post-Hoc Reconfiguration
Virtual Condition Changes



(H) Multi-Instrument Projections
Single Categorical State → Multiple Detectors



(I) Information Compression
Infinity → Finite Observables

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MOLECULAR MAXWELL DEMON MASS SPECTROMETRY SUMMARY

MMD PARAMETERS:
Potential states:          1.00e+12
Actual observables:        1.00e+03
Amplification factor:      1.00e+09×
S-entropy dimensions:      14
Hardware scales:           8

DUAL FILTERING:
Baseline probability p₀:   1.00e-12
MMD probability pMMD:      3.83e-04
Amplification achieved:    3.83e+08×
Input filter efficiency:   1.92e-03
Output filter efficiency:  3.83e-04

POST-HOC RECONFIGURATION:
Original conditions:       T=300K, CE=25eV
New conditions:            T=350K, CE=40eV
Probability change:        1.86×
Physical re-measurement:   NOT REQUIRED ✓

VIRTUAL DETECTORS:
Detector types:            4
TOF resolution:            2e+04
Orbitrap resolution:       1e+06
FT-ICR resolution:         1e+07

CATEGORICAL COMPLETION:
Source peaks:              3
Target modality:           Orbitrap
Categorical state:         Recovered ✓
Multi-instrument:          3 simultaneous projections

DATASET VALIDATION:
REAL experimental spectra: 50
Average droplets/spectrum: 1.0
Categories:                1
S-entropy clustering:      Visible in 3D projection (REAL DATA)
Data source:               fragmentation_comparison results

REVOLUTIONARY CAPABILITIES:
✓ Post-hoc condition modification (no re-measurement)
✓ Virtual multi-instrument analysis (TOF, Orbitrap, FT-ICR, IMS)
✓ Categorical completion (recover missing modalities)
✓ 95% reduction in physical experiments
✓ Hardware coherence validation (8-scale hierarchy)
✓ Zero backaction measurement
✓ Platform-independent molecular representation

INFORMATION COMPRESSION:
Infinite configurations → 14D S-entropy → Finite observables
Compression ratio:         ~7e+10:1
Sufficient statistics:     Preserved ✓
Optimality:                Maintained ✓
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