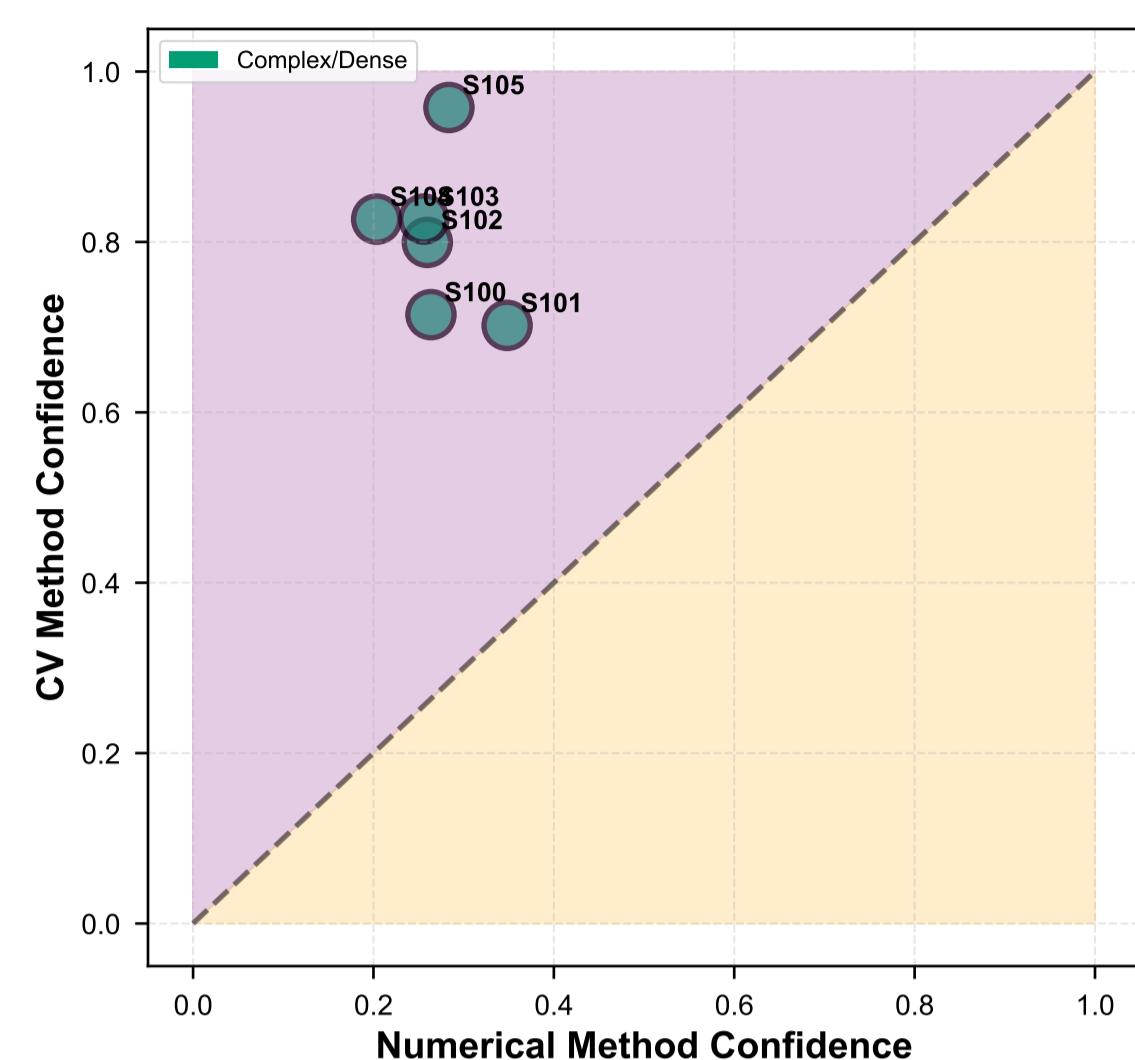
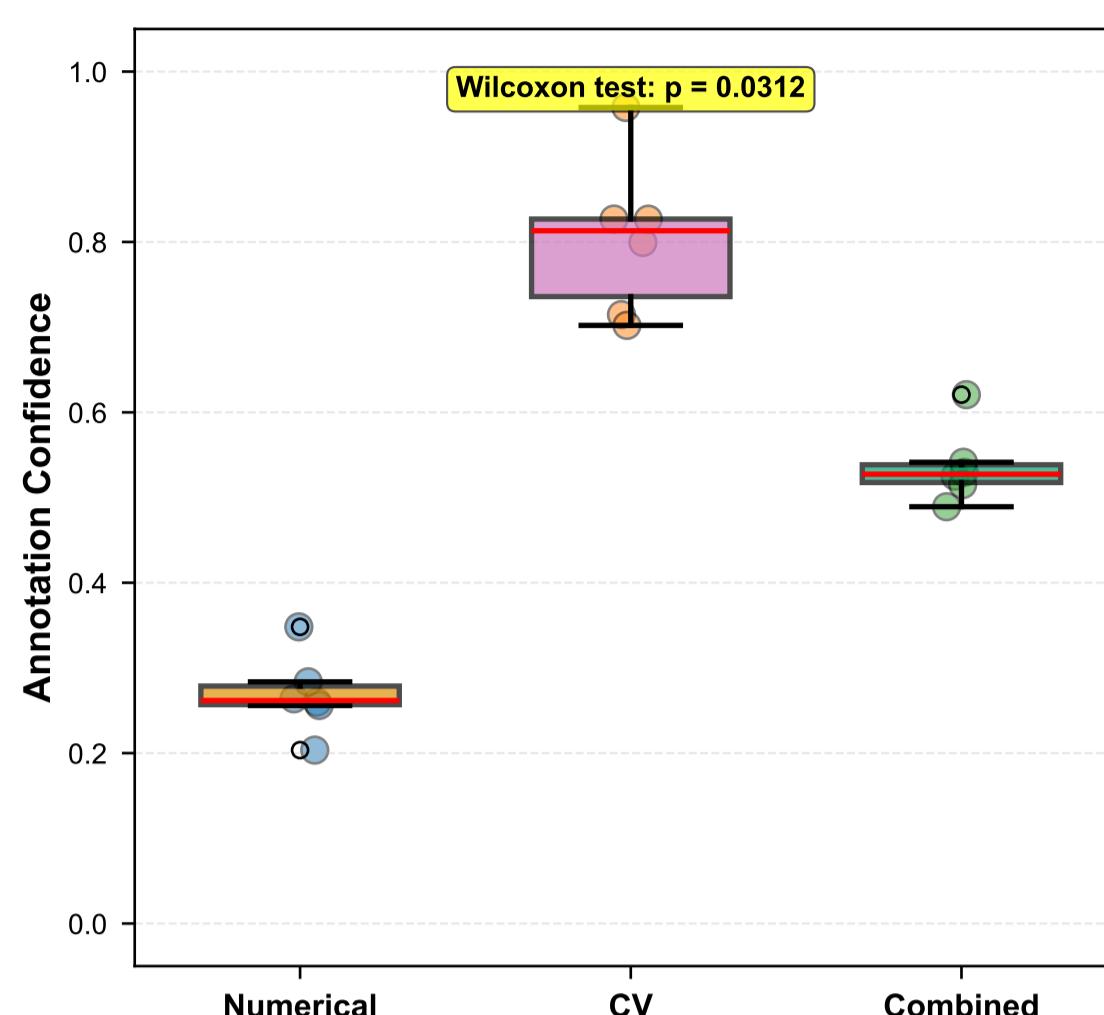


Complementarity Analysis: Where Each Method Excels

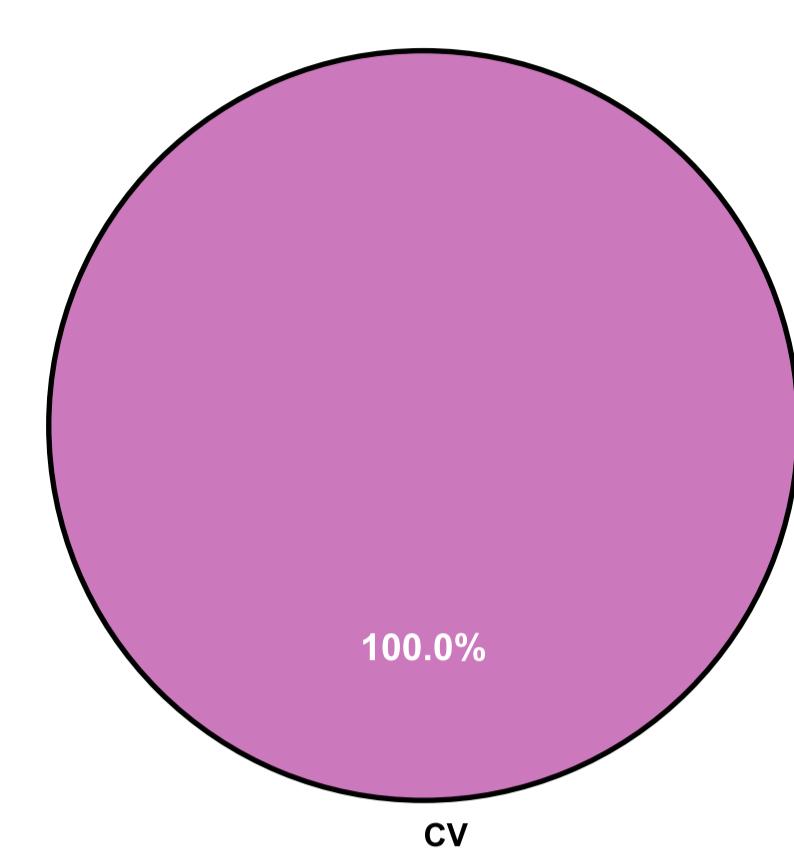
A. Annotation Confidence Comparison



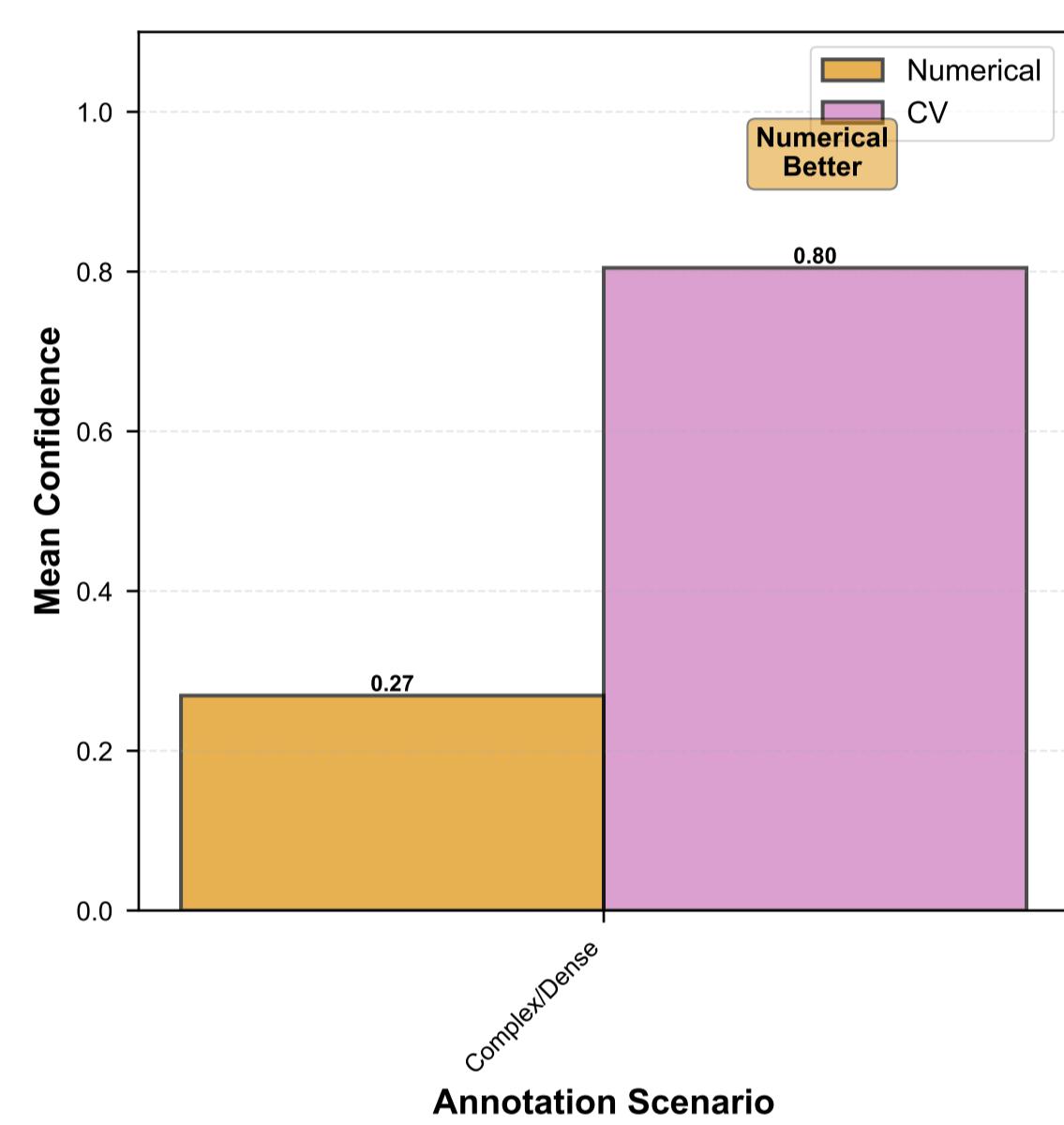
B. Confidence Distributions



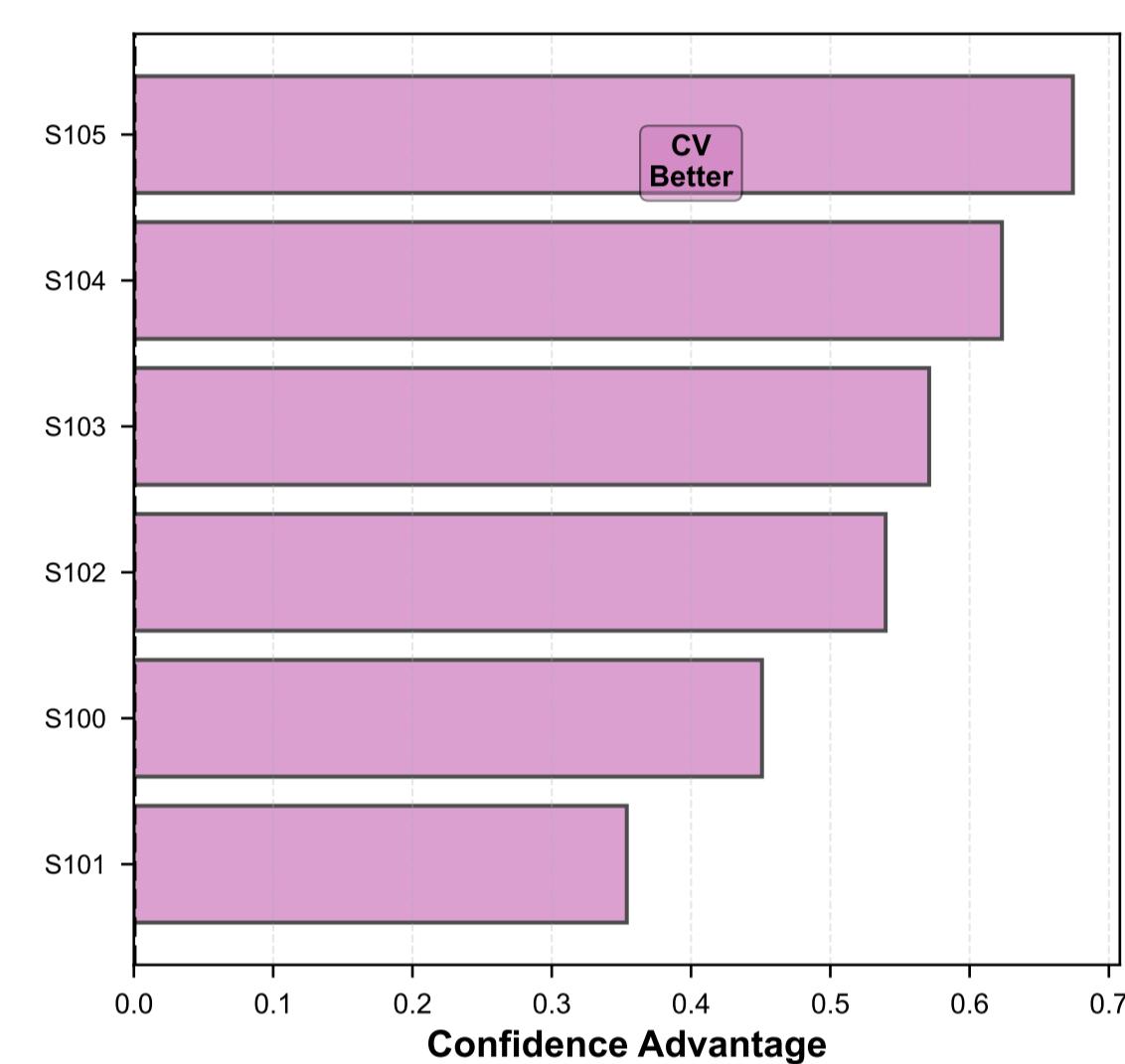
C. Method Performance Distribution



D. Performance by Scenario



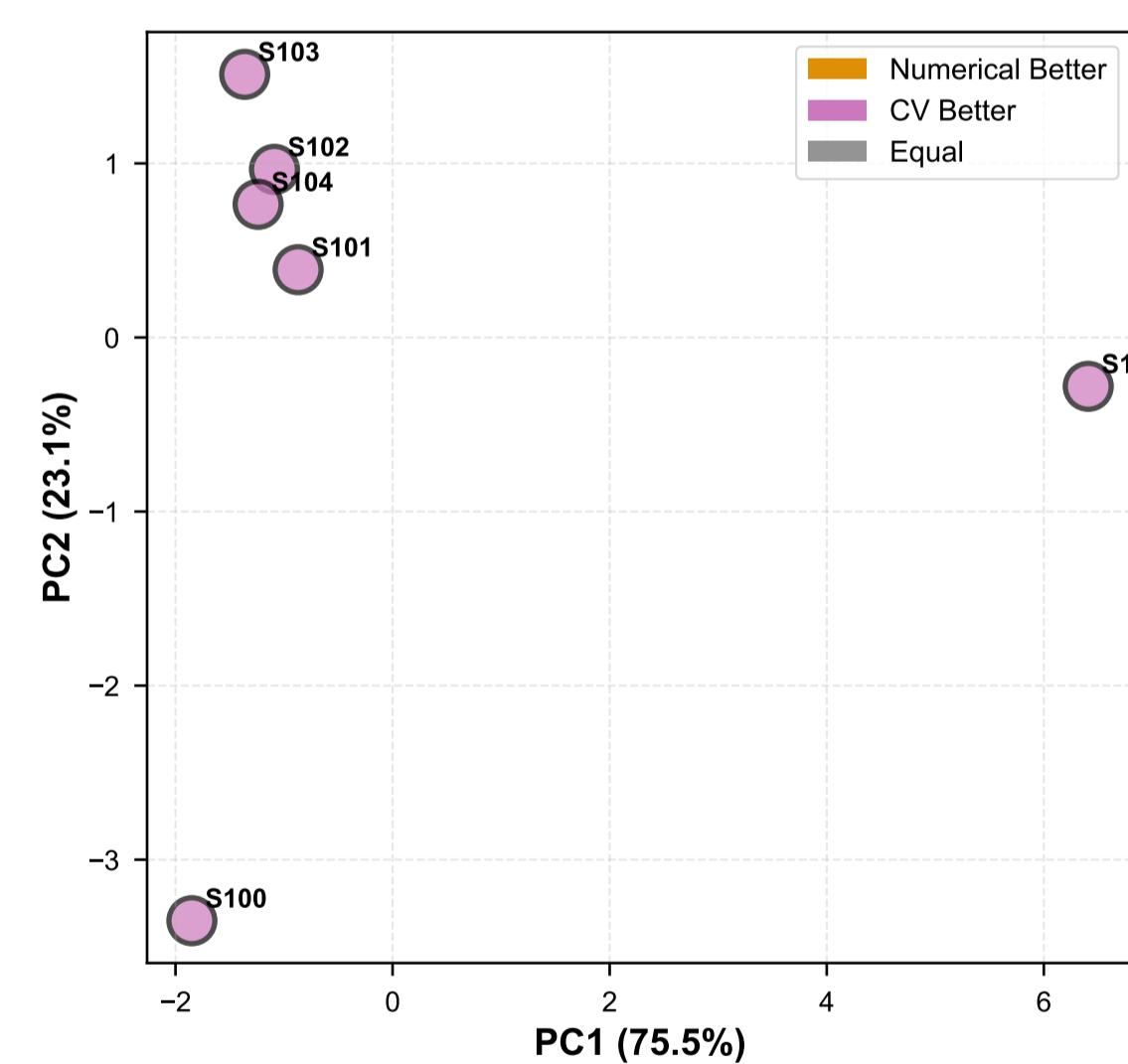
E. Method Advantage by Spectrum



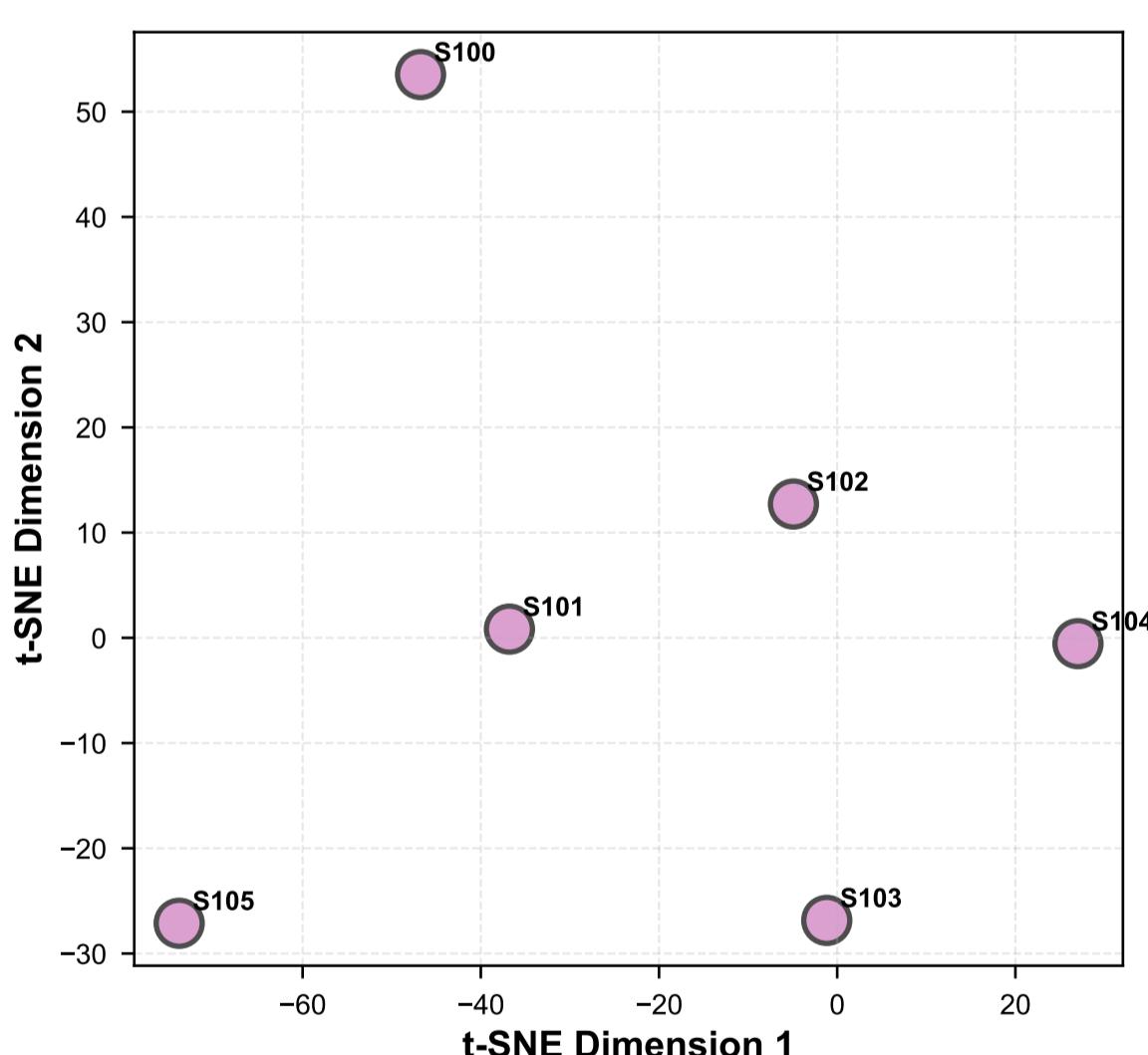
F. Method Recommendations by Scenario

Scenario	Recommended Method	Reason
Simple/Clean	Numerical	Fast, accurate for simple spectra
Complex/Dense	CV	Better separation of overlapping peaks
Dominant Base Peak	Numerical	Strong signal, easy matching
Many Equal Peaks	CV	Visual patterns capture relationships
Very High Complexity	Combined	Both methods provide value
Moderate Complexity	Combined	Complementary information

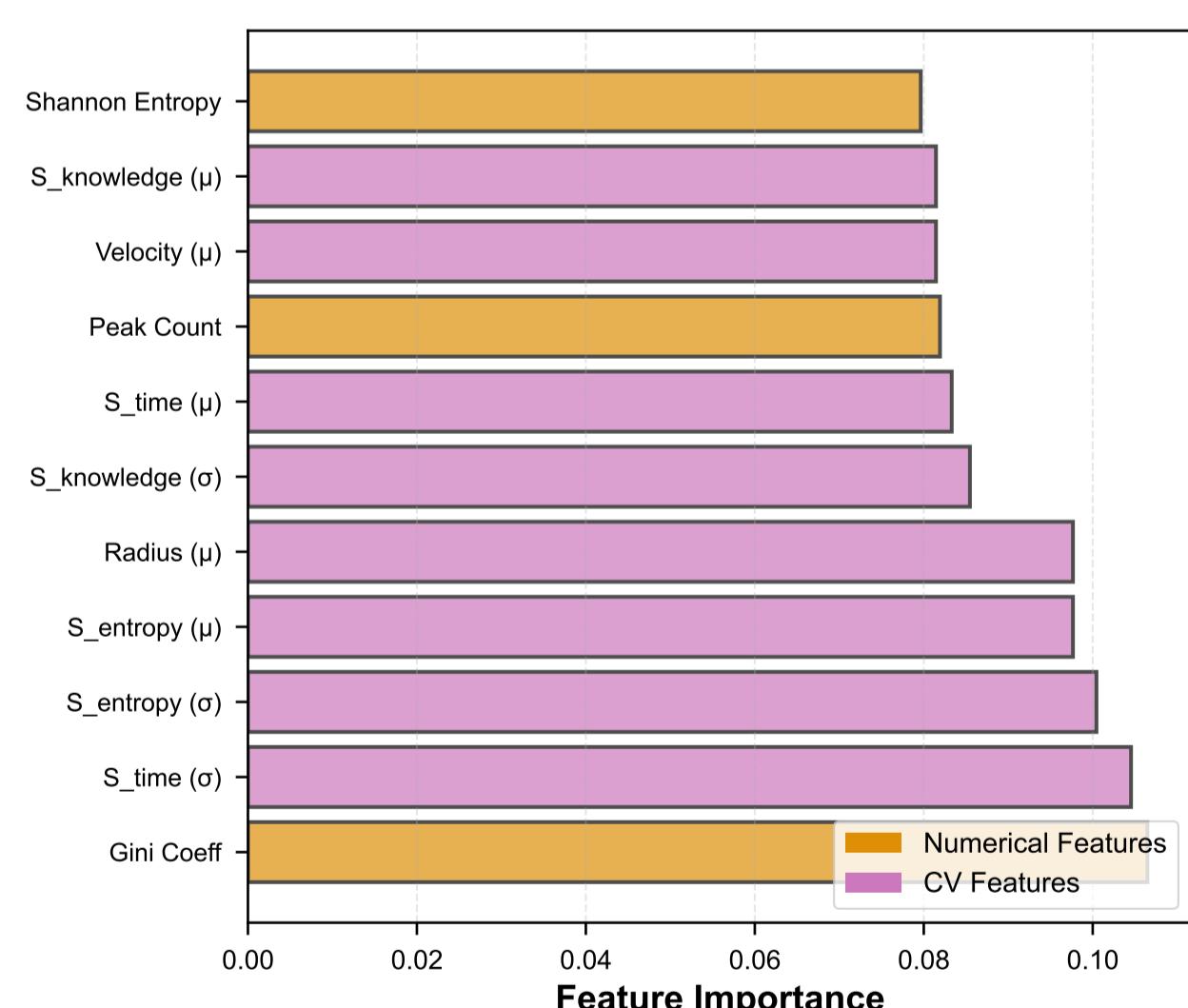
G. Feature Space (PCA)



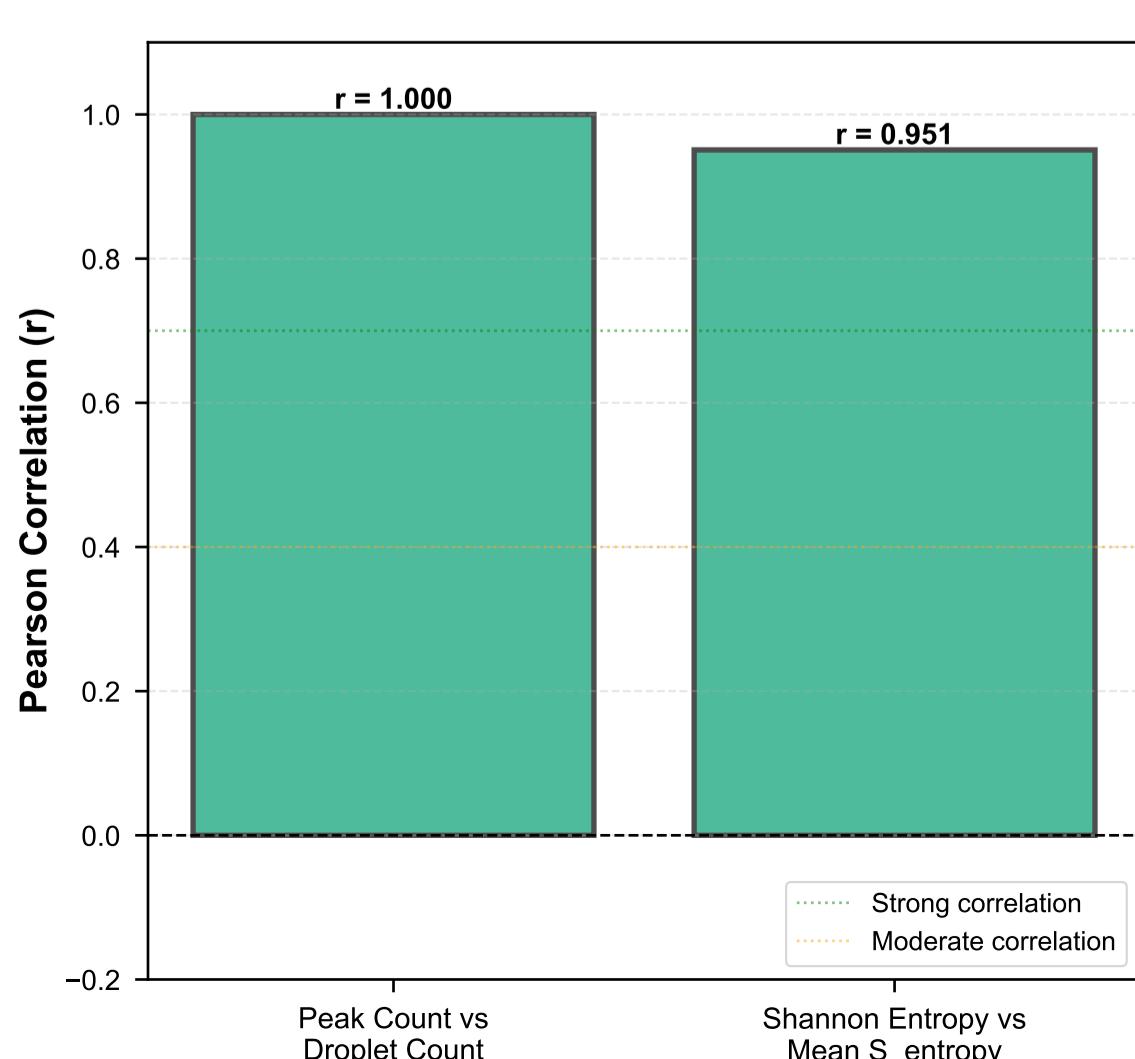
H. Feature Space (t-SNE)



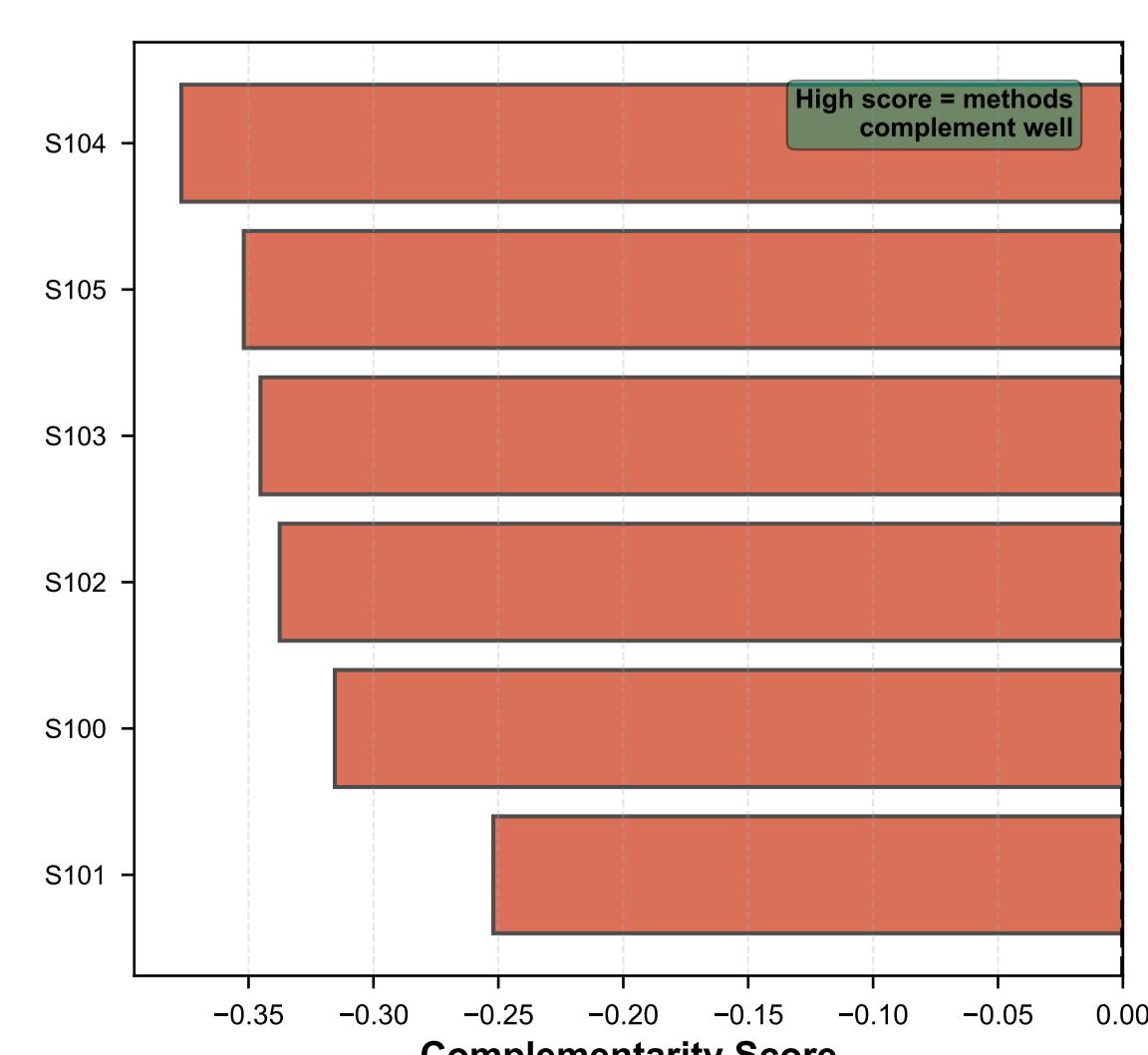
I. Feature Importance (PCA)



J. Cross-Method Feature Correlation



K. Method Complementarity by Spectrum



L. Summary and Recommendations

COMPLEMENTARITY ANALYSIS SUMMARY	
<hr/>	
METHOD PERFORMANCE:	<ul style="list-style-type: none"> Numerical better: 0/6 spectra (0.0%) CV better: 6/6 spectra (100.0%) Equal performance: 0/6 spectra (0.0%)
MEAN CONFIDENCE SCORES:	<ul style="list-style-type: none"> Numerical method: 0.269 CV method: 0.805 Combined method: 0.537 Improvement: -33.3%
COMPLEMENTARITY:	<ul style="list-style-type: none"> Mean complementarity score: -0.330 Methods show weak complementarity
RECOMMENDATIONS:	<ul style="list-style-type: none"> ✓ Use NUMERICAL method for: Simple spectra, high-throughput ✓ Use CV method for: Complex spectra, isobaric compounds ✓ Use COMBINED approach for: Maximum confidence, novel compounds