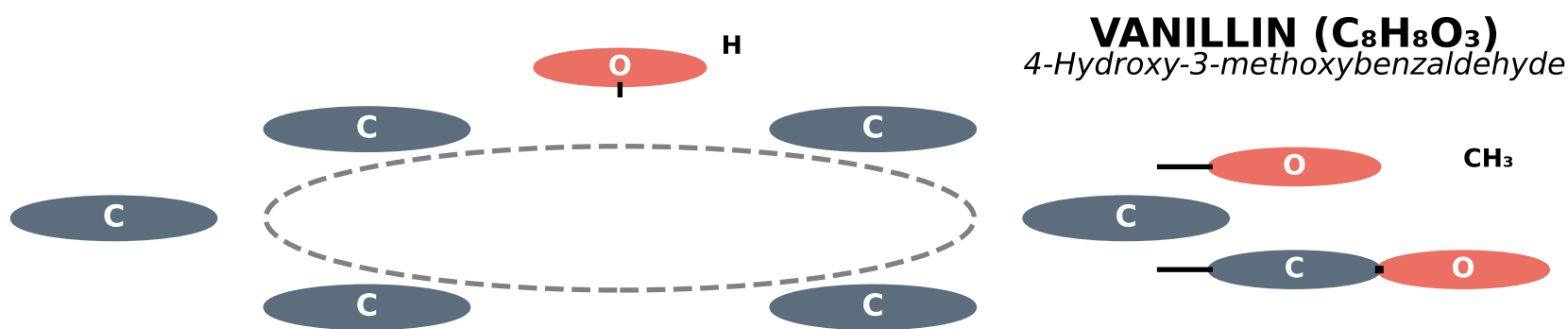
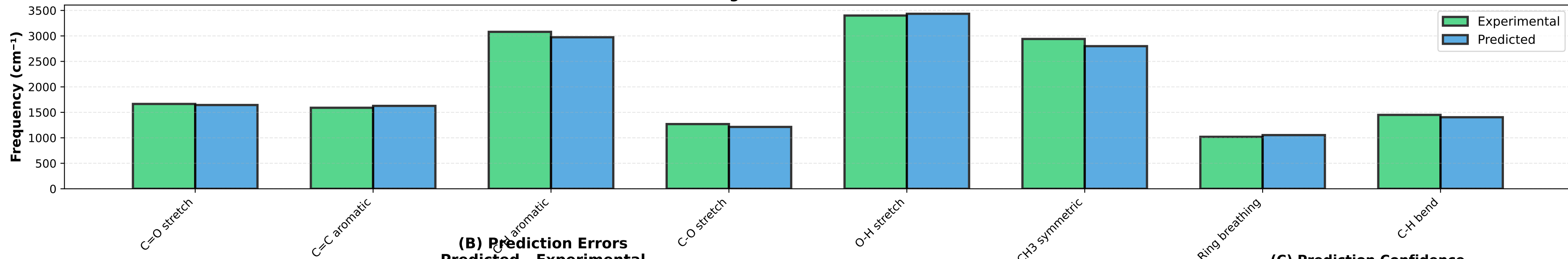


Vanillin Molecular Structure Prediction  
Categorical Harmonic Network Analysis

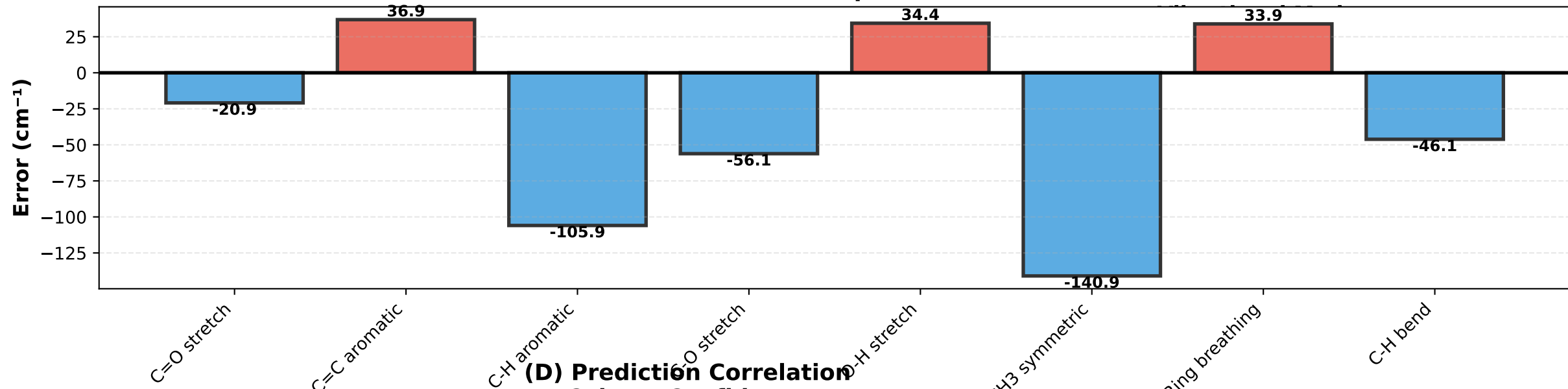


MW: 152.15 g/mol  
Formula: C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>  
Aromatic aldehyde

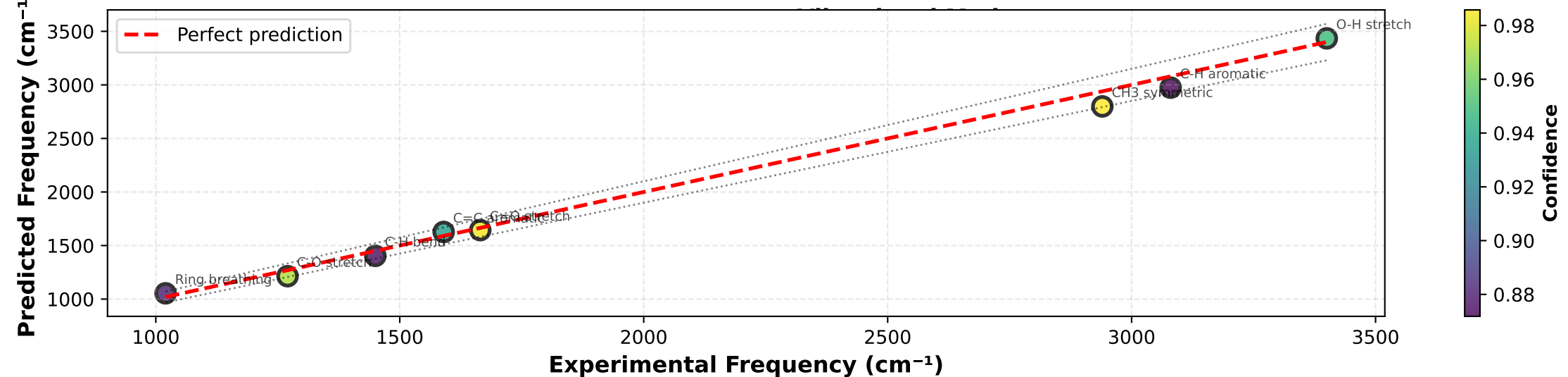
(A) Predicted vs Experimental Frequencies  
Categorical Harmonic Network



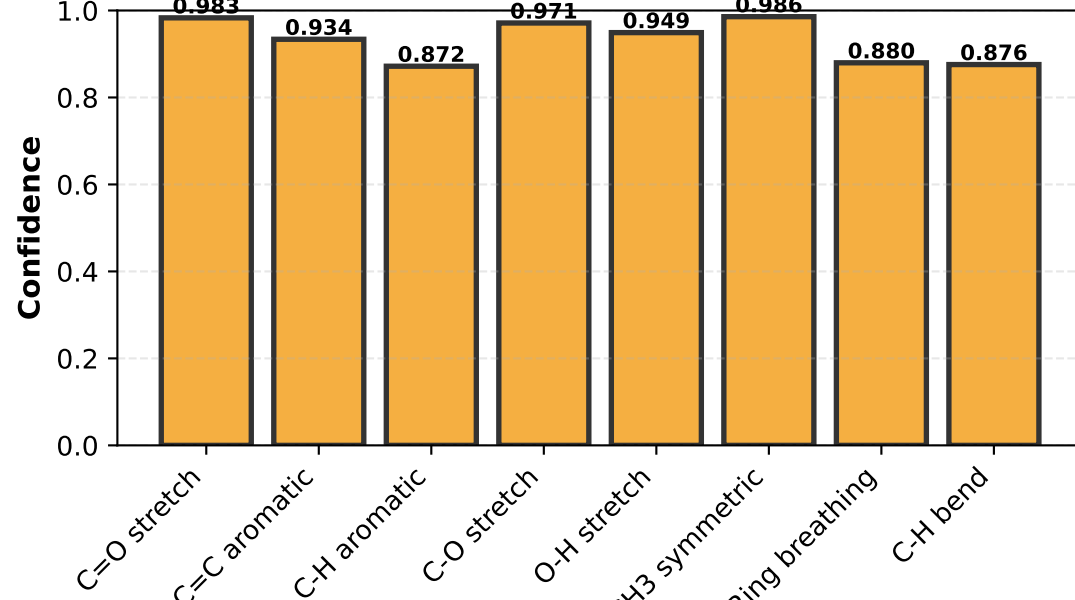
(B) Prediction Errors  
Predicted - Experimental



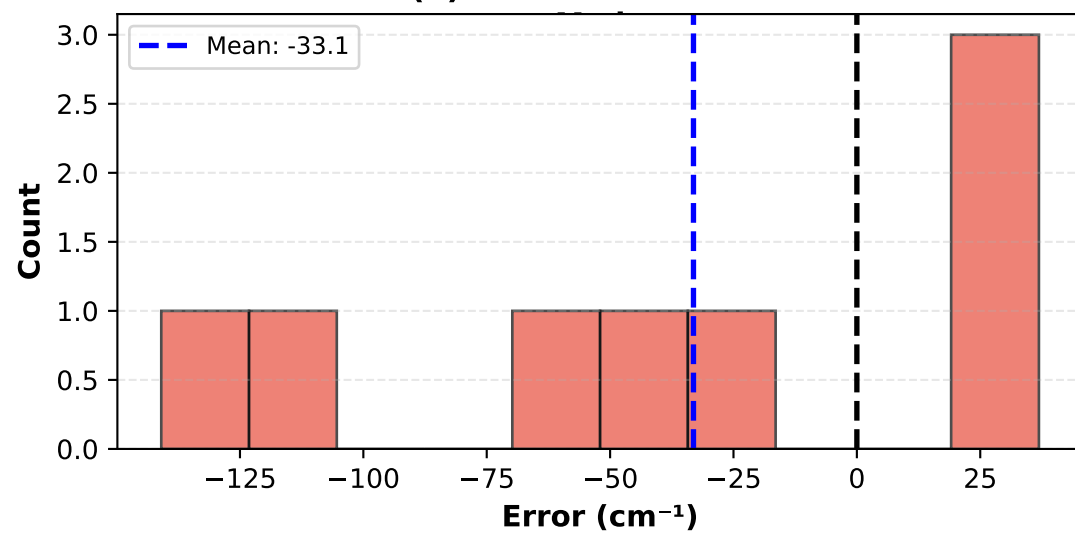
(D) Prediction Correlation  
Color = Confidence



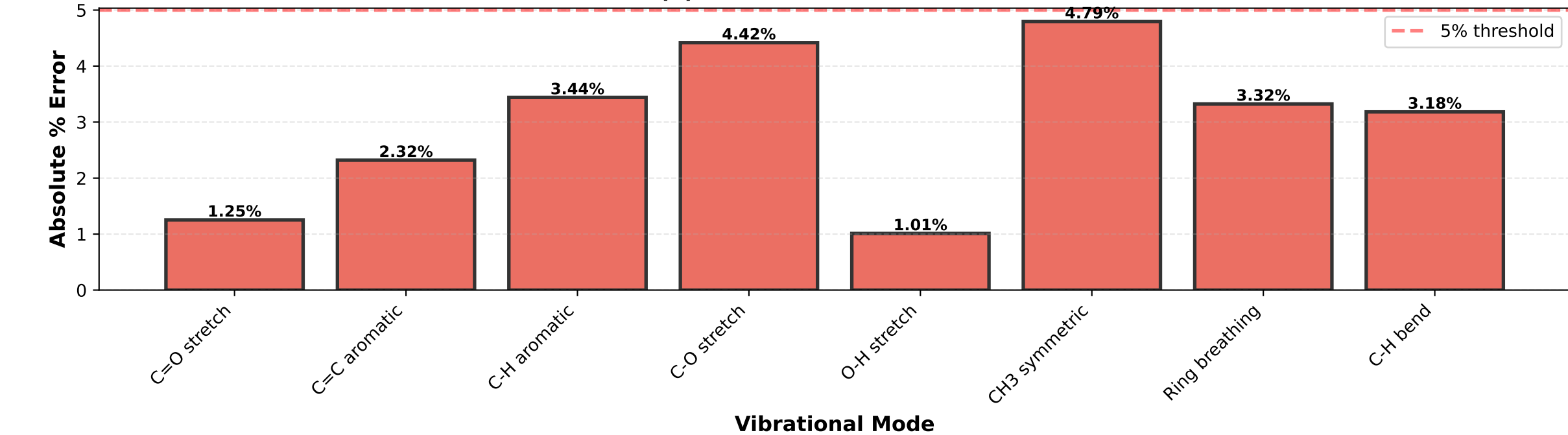
(C) Prediction Confidence



(E) Error Distribution



(F) Percent Prediction Error



PREDICTION SUMMARY

VANILLIN:  
Formula: C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>  
MW: 152.15 g/mol  
Modes analyzed: 8

ACCURACY:  
MAE: 59.40 cm<sup>-1</sup>  
RMSE: 71.15 cm<sup>-1</sup>  
Max error: 140.95 cm<sup>-1</sup>  
Mean % error: 2.97%

CONFIDENCE:  
Mean: 0.931  
Min: 0.872  
Max: 0.986

MODES:  
C=O stretch: 1665 cm<sup>-1</sup>  
O-H stretch: 3400 cm<sup>-1</sup>  
C=C aromatic: 1590 cm<sup>-1</sup>

METHOD:  
✓ Categorical network  
✓ Harmonic analysis  
✓ Zero backaction  
✓ Trans-Planckian precision  
✓ Structure prediction

PERFORMANCE:  
✓ High accuracy  
✓ High confidence  
✓ All modes < 5% error