Supporting Information:

Similarity in Dissymmetry Factor Spectra: A Quantitative Measure of Comparison between Experimental and Predicted Vibrational Circular Dichroism

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Figure S1. Influence of bandwidth on dissymmetry factor spectra for overlapping bands. Two bands at 1060 and 1040 cm^{-1} were simulated with 3, 5, 10 cm^{-1} HWHM.

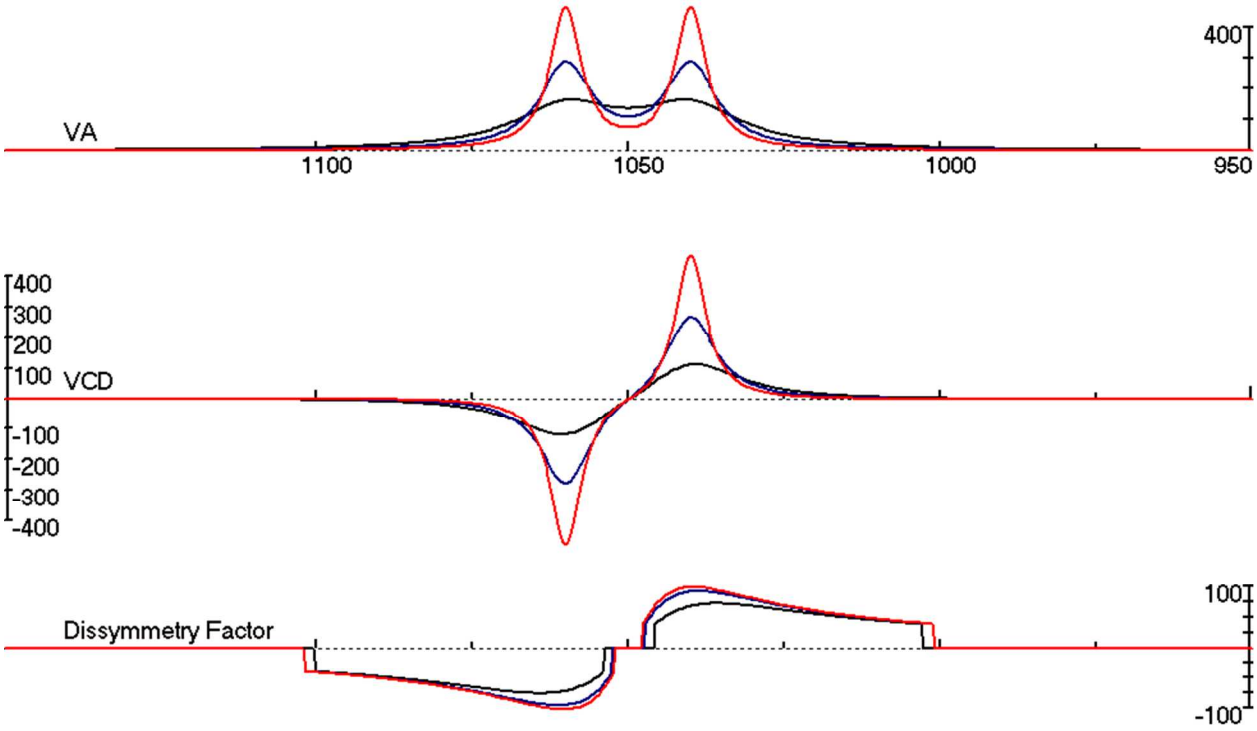

Figure S2. Influence of bandwidth on dissymmetry factor spectra for strongly overlapping C=O stretching bands of dimethyl tartrate: Absorption (top), VCD (middle) and dissymmetry factor (bottom) traces in experimental (left) and calculated spectra. Note that when 3 cm^{-1} half-width at half-maximum (HWHM) is used the calculated dissymmetry factors come above the robustness criterion but when 5 cm^{-1} bandwidth is used the dissymmetry factors fall below the robust criterion.

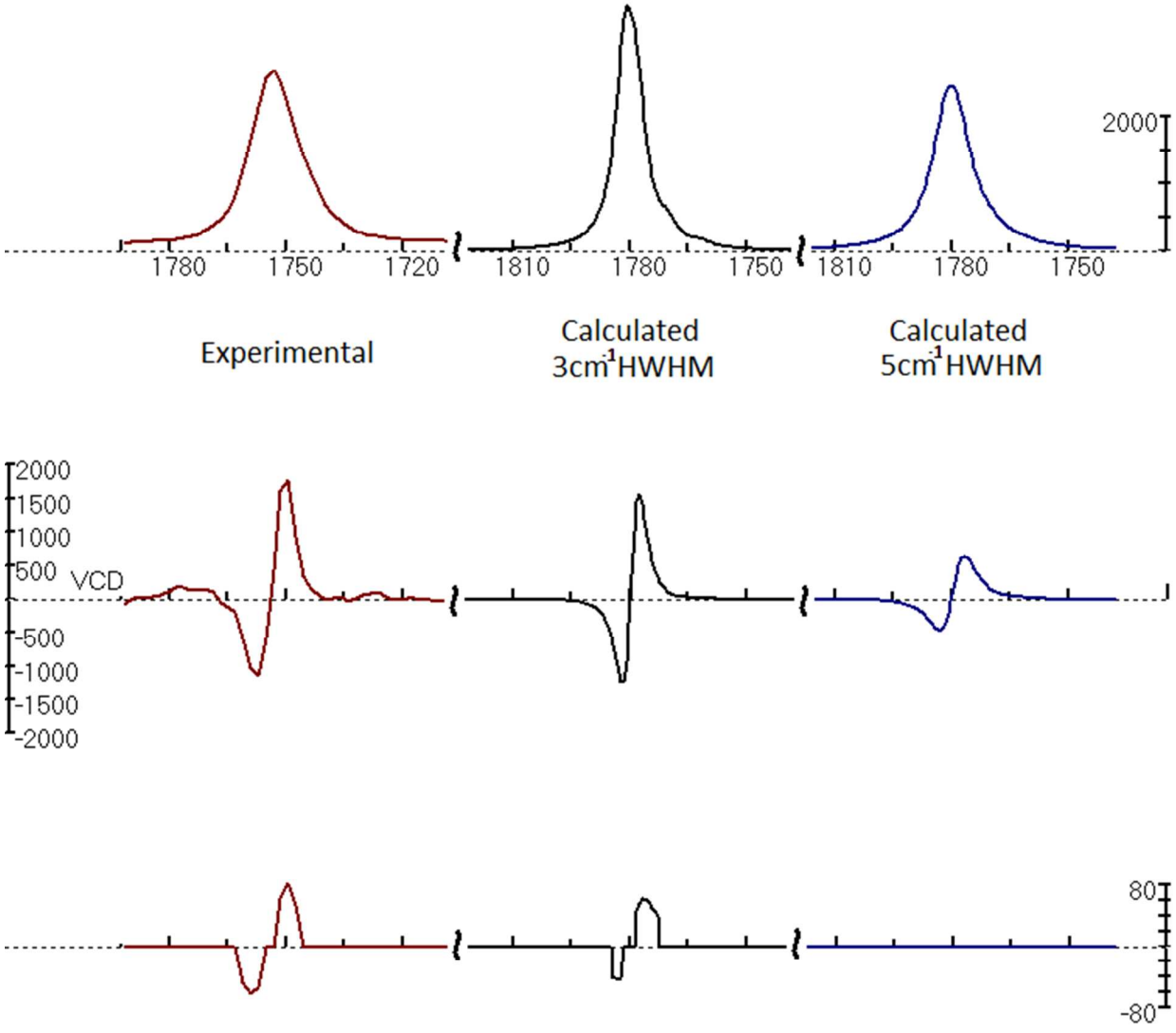

Figure S3: ESI Calculations for (R)-(+)-3-chloro-1-butyne

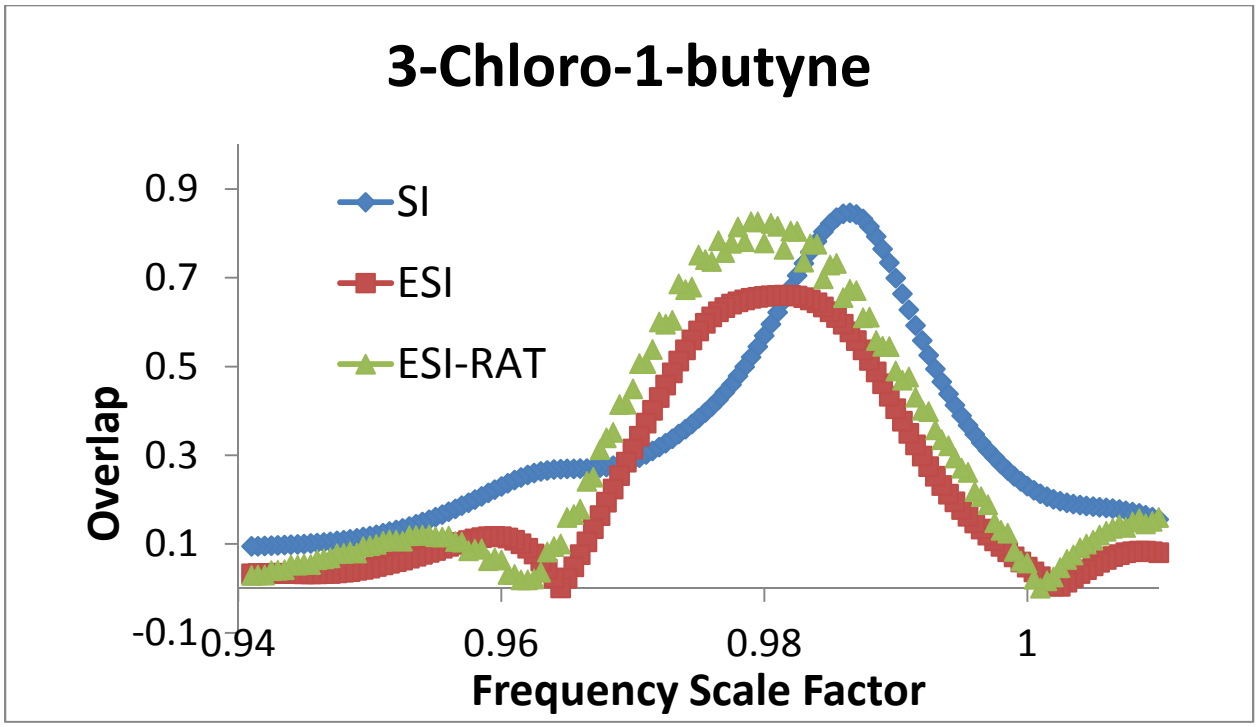

Figure S4: ESI Calculations for (3R)-(+)-methylcyclopentanone

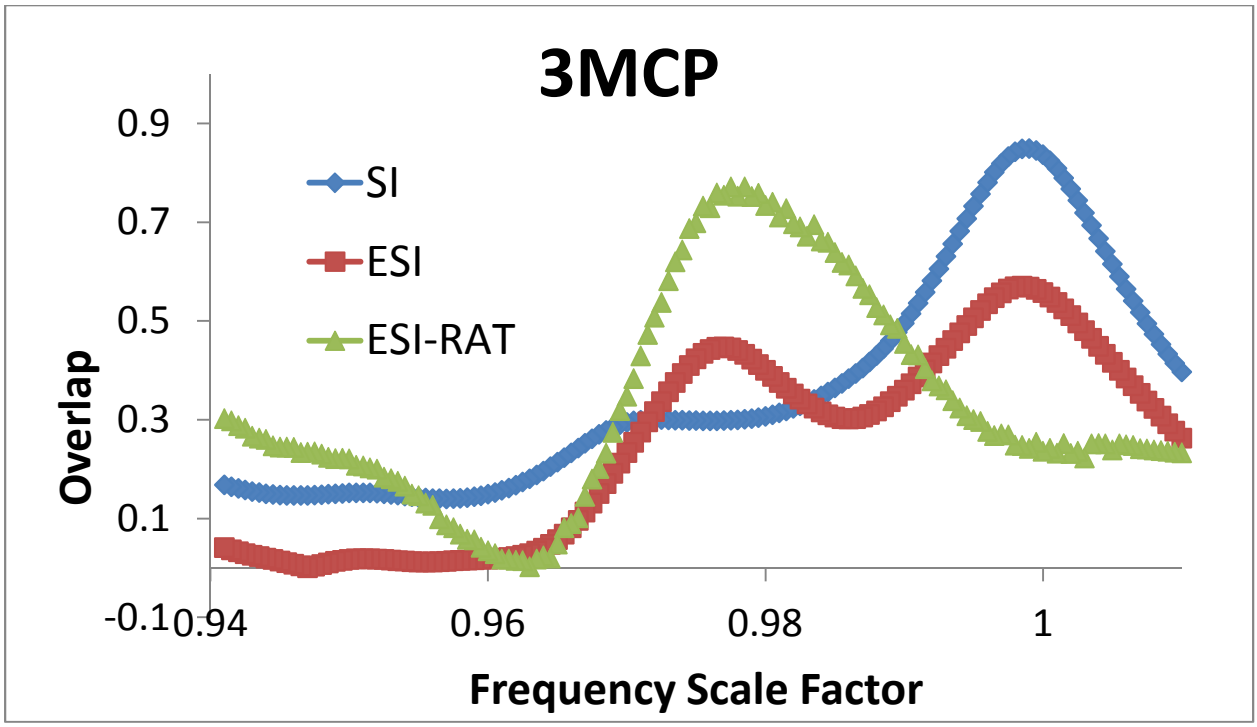

Figure S5: ESI Calculations for (1*S*)-(-)-α -pinene

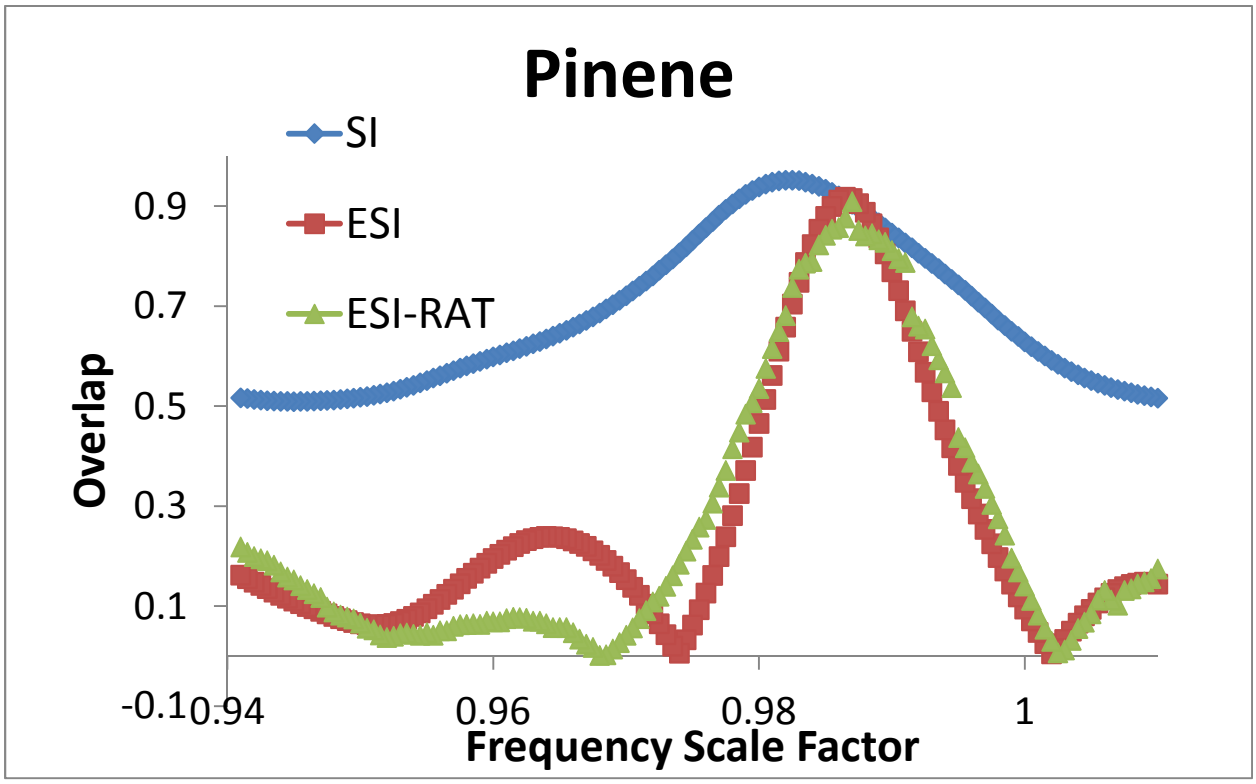

Figure S6: ESI Calculations for (3R)-(+)--methylcyclohexanone

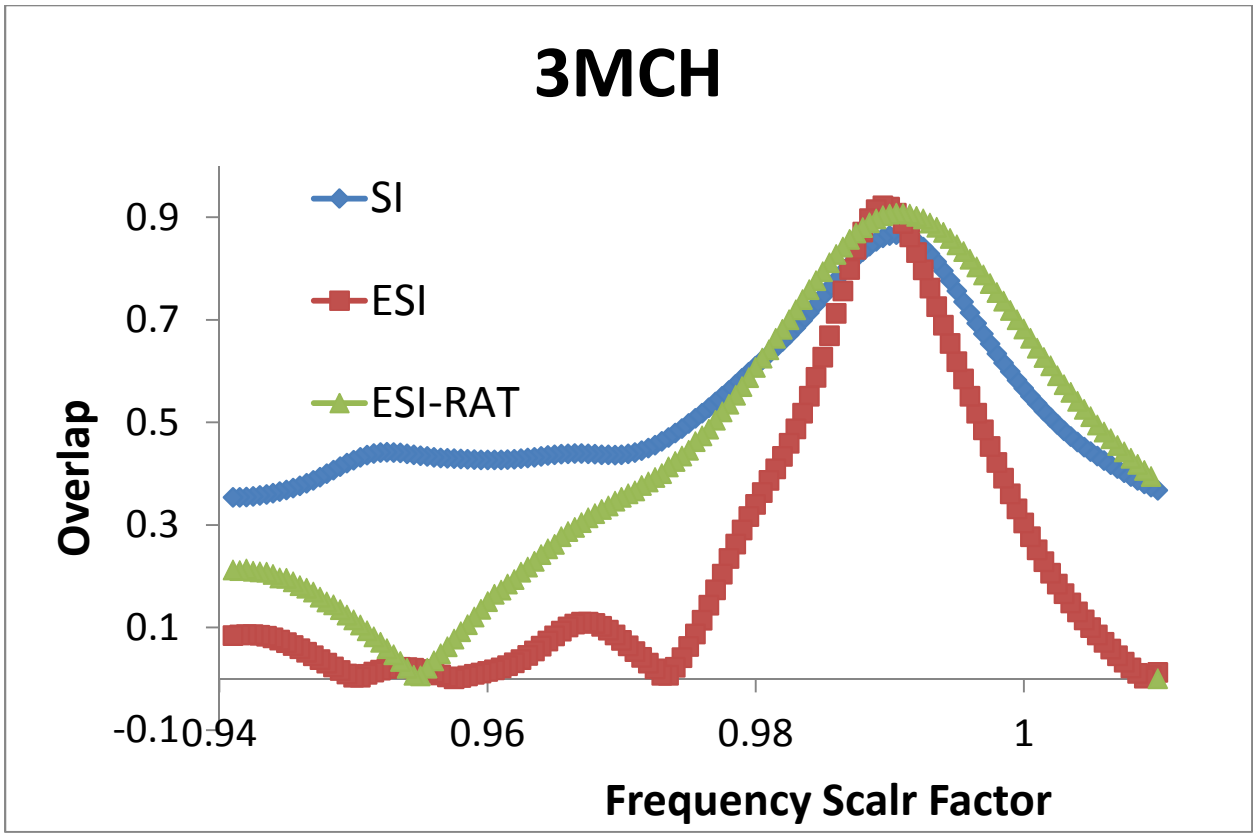

Figure S7: ESI Calculations for (1R)-(+)-camphor

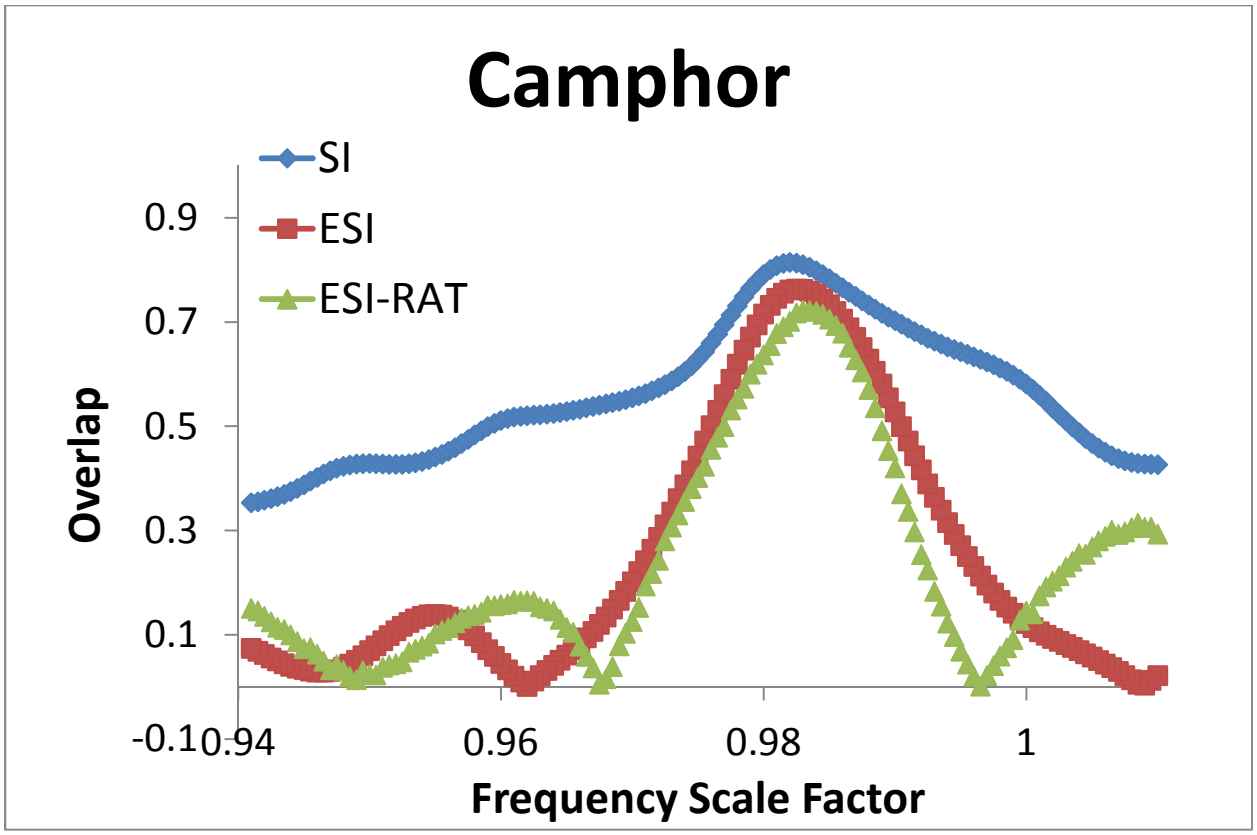

Figure S8: ESI Calculations for(S)-(+)-epichlorohydrin

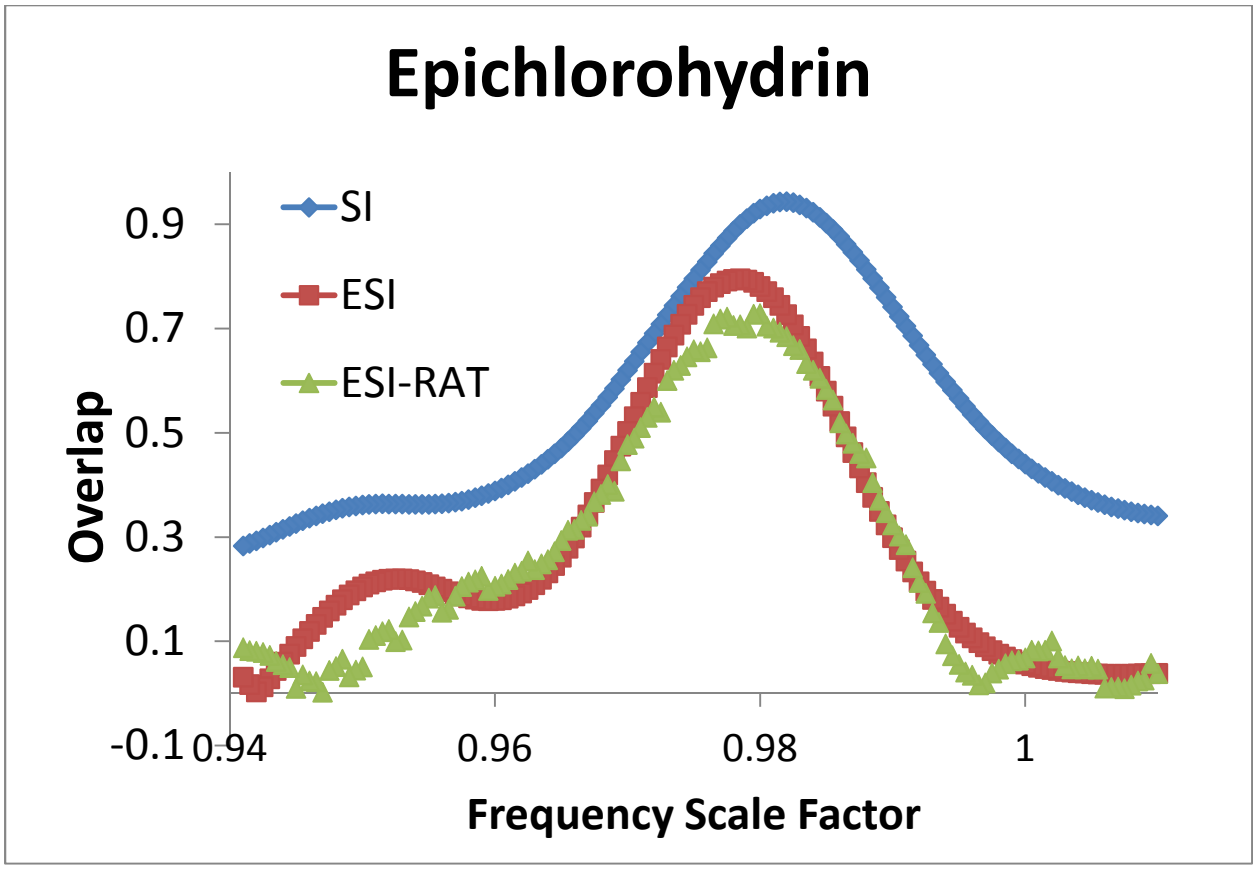

Figure S9: ESI Calculations for overlap between experimental spectra of -α-pinene and calculated spectra for 3-methylcyclopentanone.