

SUPPORTING INFORMATION

Improving the IR Spectra Alignment Algorithm with Spectra Deconvolution and Combination with Raman or VCD Spectroscopy

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1 Isomer Definition

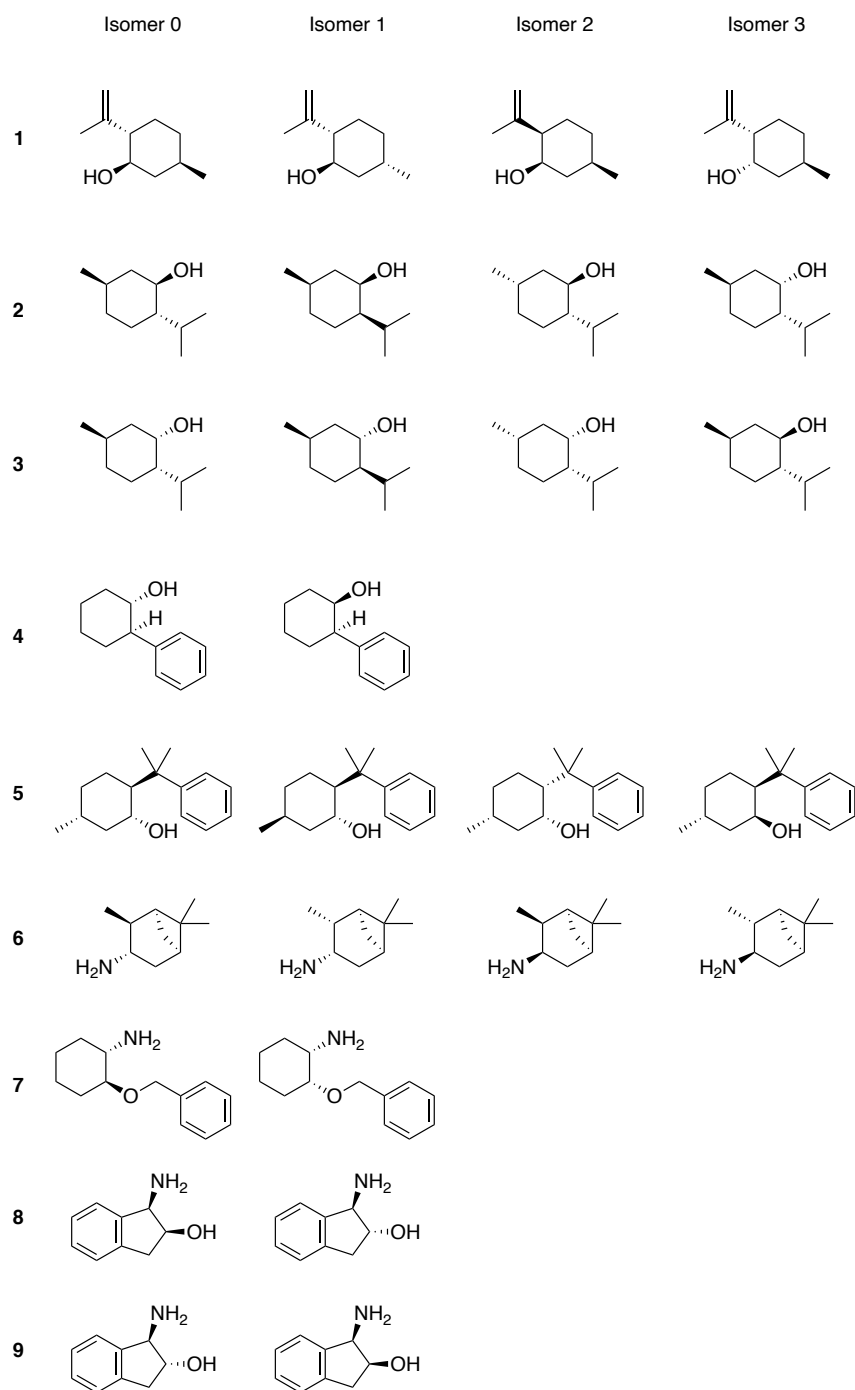


Figure S1: Isomer definition used for compounds 1-9.

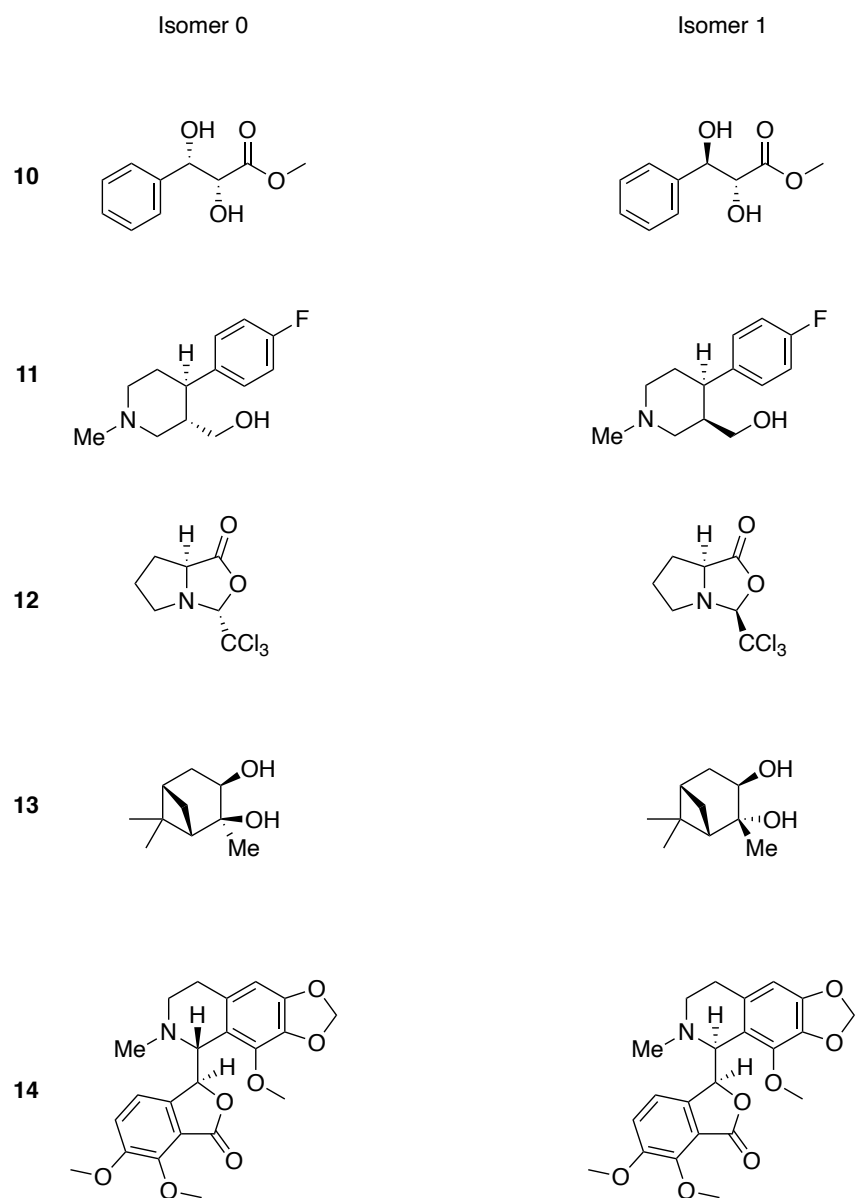


Figure S2: Isomer definition used for compounds 10-14.

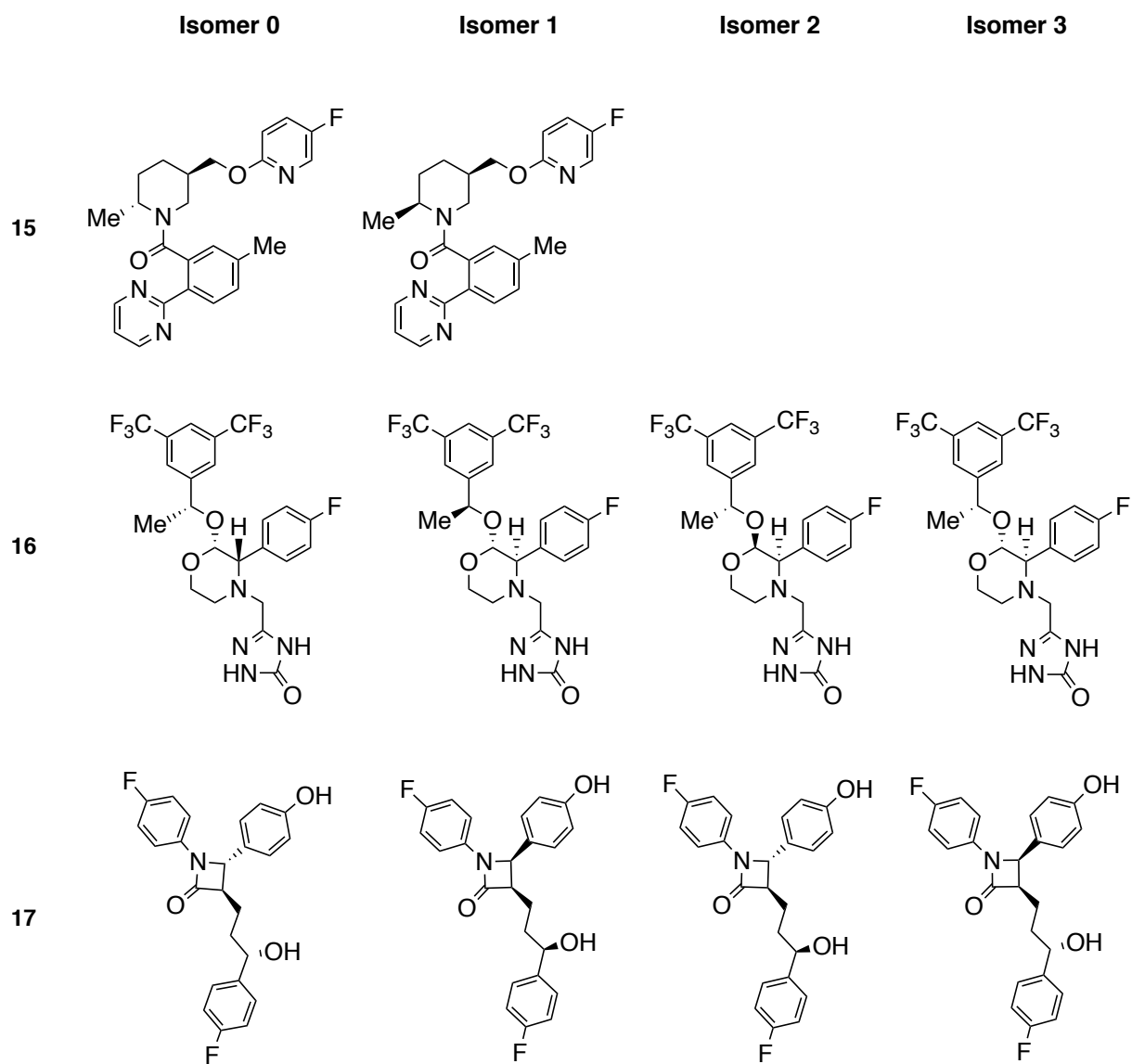


Figure S3: Isomer definition used for compounds **15-17**.

2 Correlation Plots

2.1 Compound 2

2.1.1 Alignment Alignment Score s and Combined Score

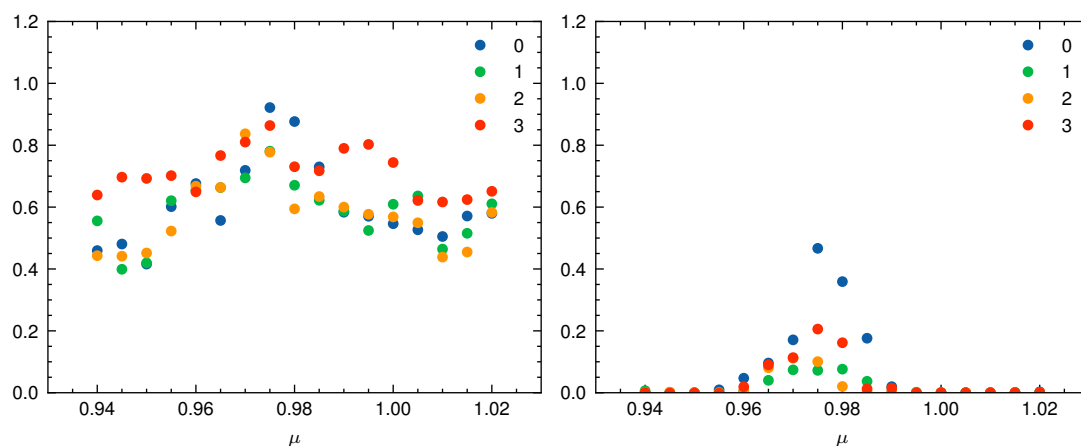


Figure S4: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **2**: total alignment score s (left) and combined score s_{comb} (right).

2.1.2 Pearson Correlation Coefficient

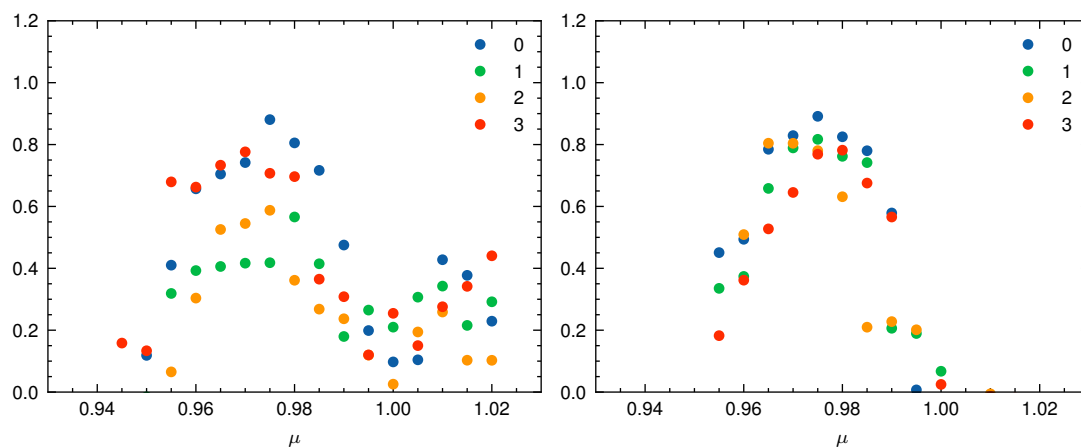


Figure S5: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **2**: Pearson correlation coefficient for IR (left) and Raman (right).

2.1.3 Spearman Correlation Coefficient

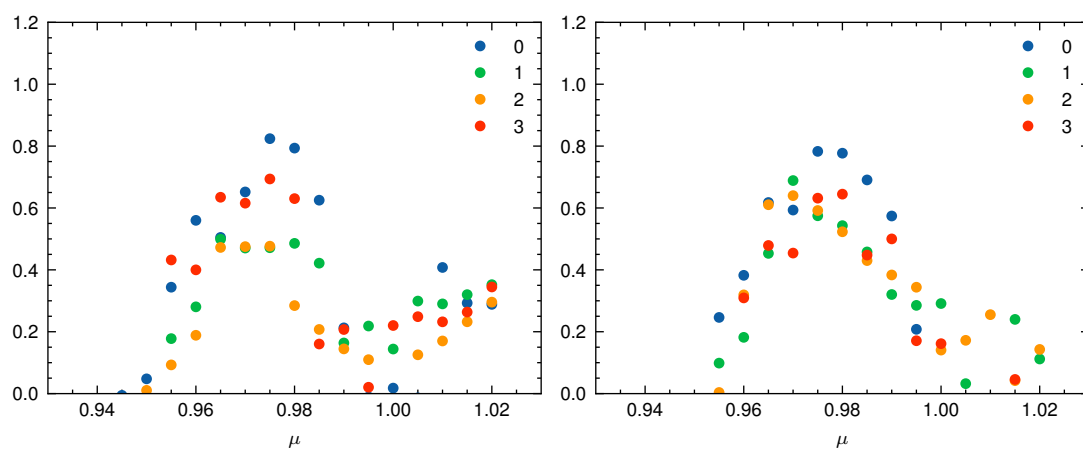


Figure S6: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **2**: Spearman correlation coefficient for IR (left) and Raman (right).

2.2 Compound 3

2.2.1 Alignment Score s and Combined Score

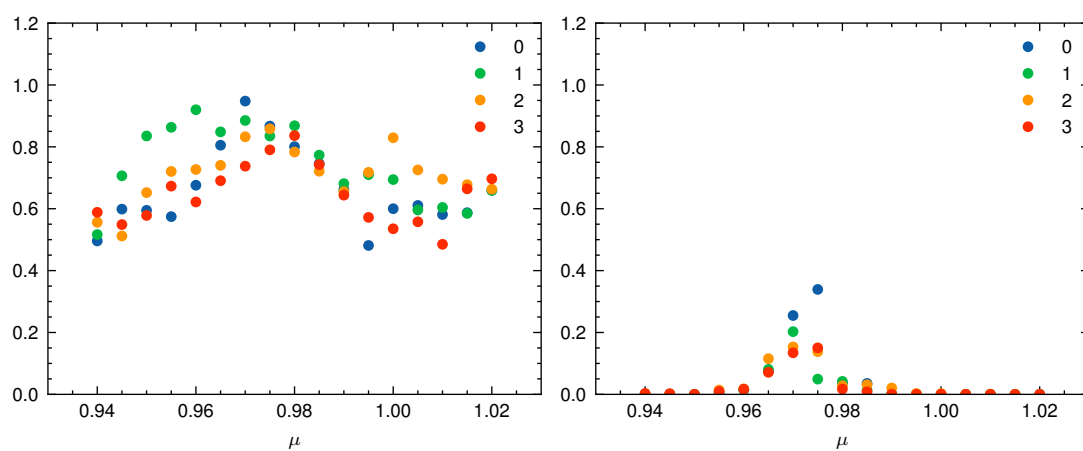


Figure S7: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **3**: total alignment score s (left) and combined score s_{comb} (right).

2.2.2 Pearson Correlation Coefficient

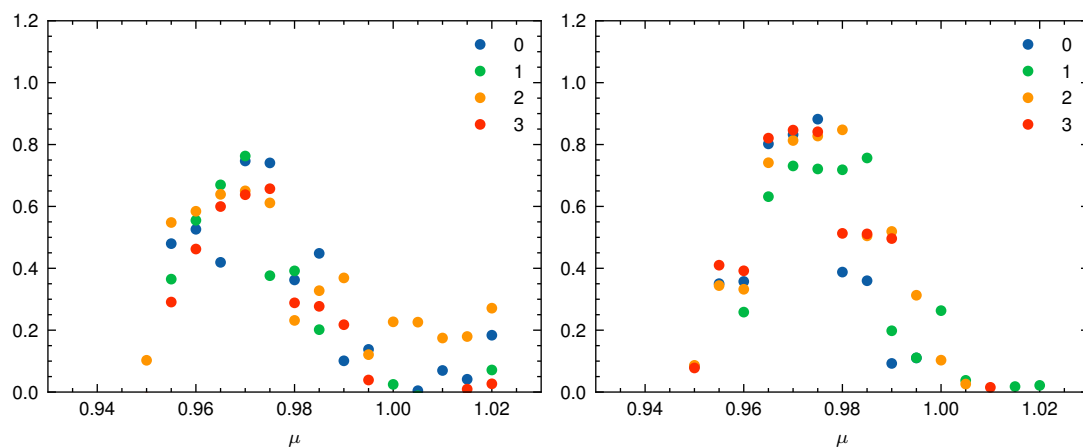


Figure S8: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **3**: Pearson correlation coefficient for IR (left) and Raman (right).

2.2.3 Spearman Correlation Coefficient

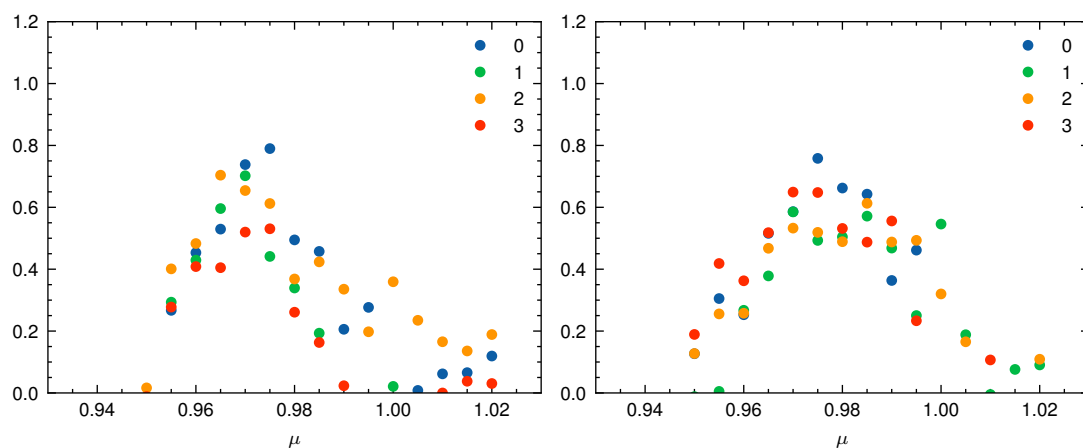


Figure S9: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **3**: Spearman correlation coefficient for IR (left) and Raman (right).

2.3 Compound 4

2.3.1 Alignment Score s and Combined Score

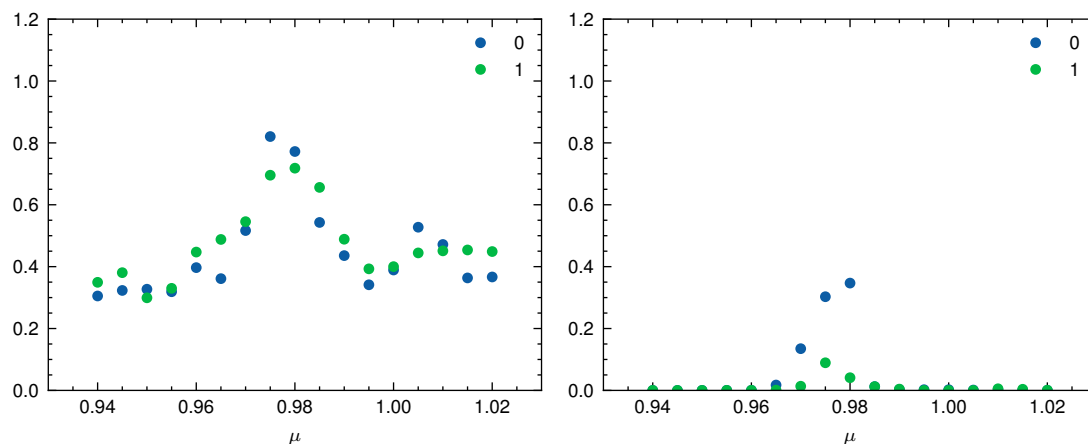


Figure S10: Evaluation metrics as a function of the scaling factor μ for the isomers of compound 4: total alignment score s (left) and combined score s_{comb} (right).

2.3.2 Pearson Correlation Coefficient

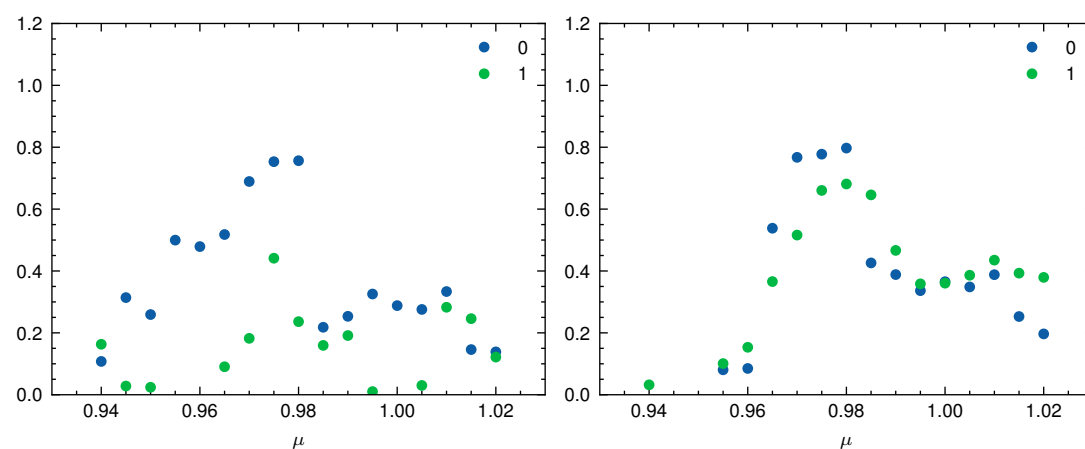


Figure S11: Evaluation metrics as a function of the scaling factor μ for the isomers of compound 4: Pearson correlation coefficient for IR (left) and Raman (right).

2.3.3 Spearman Correlation Coefficient

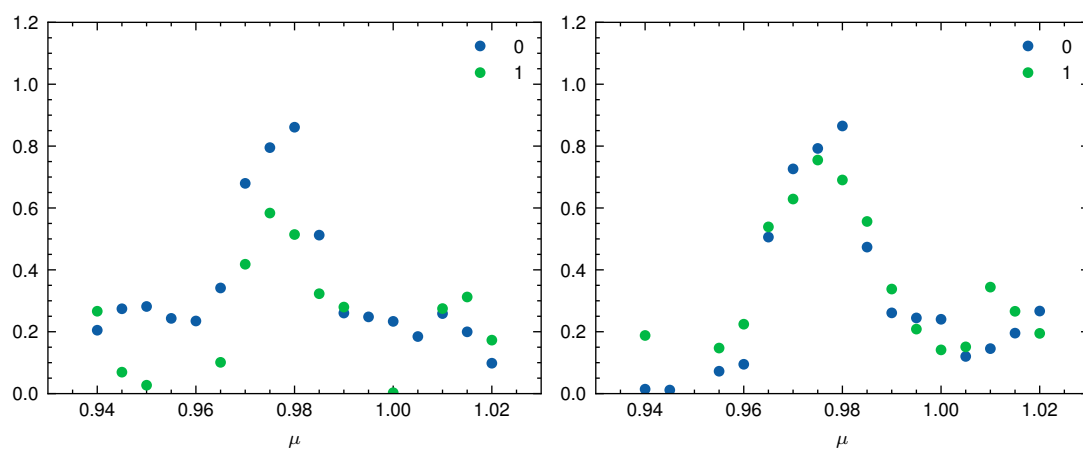


Figure S12: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **4**: Spearman correlation coefficient for IR (left) and Raman (right).

2.4 Compound 5

2.4.1 Alignment Score s and Combined Score

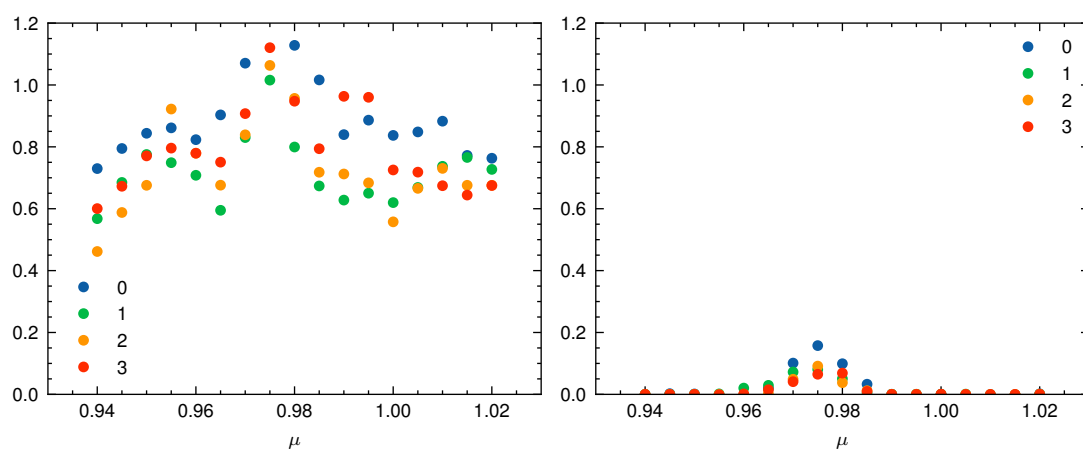


Figure S13: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **5**: total alignment score s (left) and combined score s_{comb} (right).

2.4.2 Pearson Correlation Coefficient

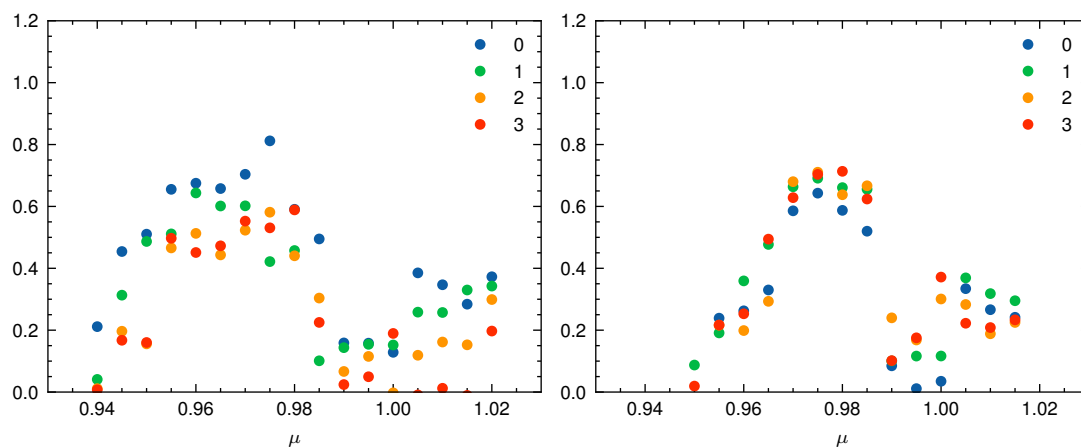


Figure S14: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **5**: Pearson correlation coefficient for IR (left) and Raman (right).

2.4.3 Spearman Correlation Coefficient

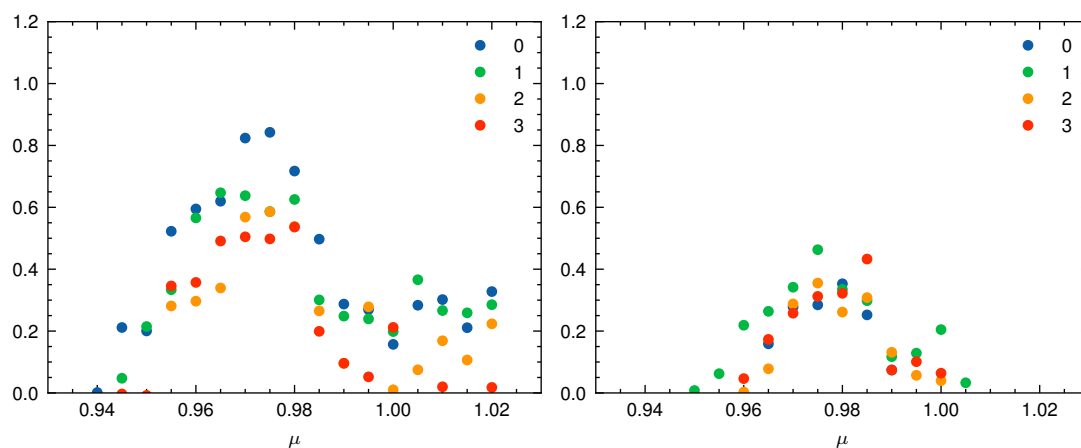


Figure S15: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **5**: Spearman correlation coefficient for IR (left) and Raman (right).

2.5 Compound 6

2.5.1 Alignment Score s and Combined Score

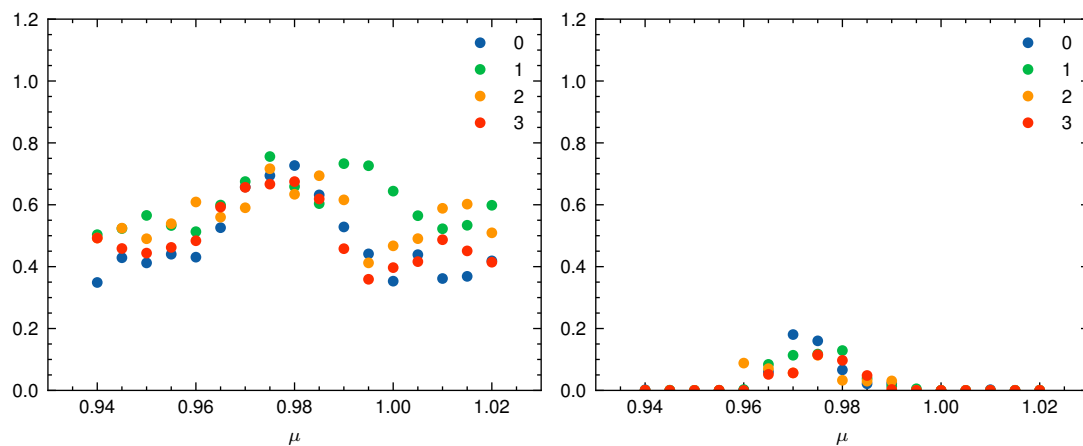


Figure S16: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **6**: total alignment score s (left) and combined score s_{comb} (right).

2.5.2 Pearson Correlation Coefficient

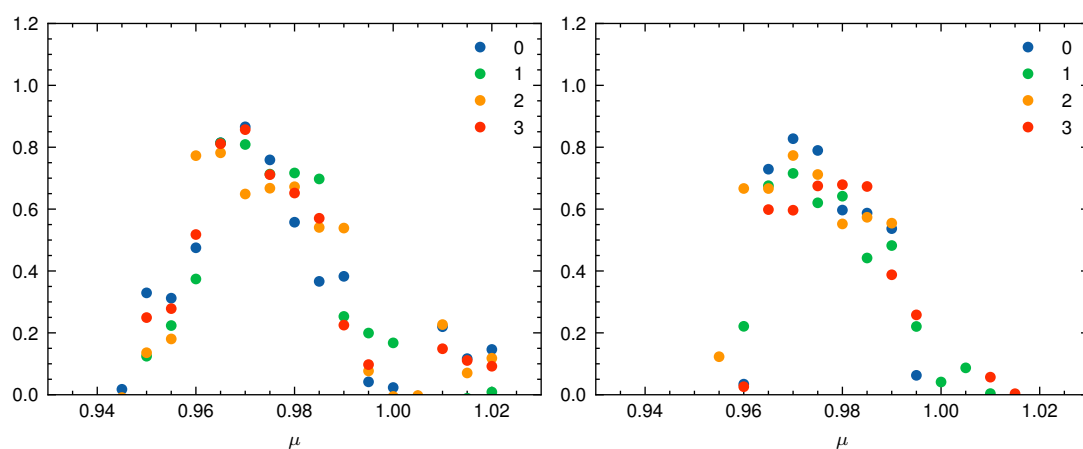


Figure S17: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **6**: Pearson correlation coefficient for IR (left) and Raman (right).

2.5.3 Spearman Correlation Coefficient

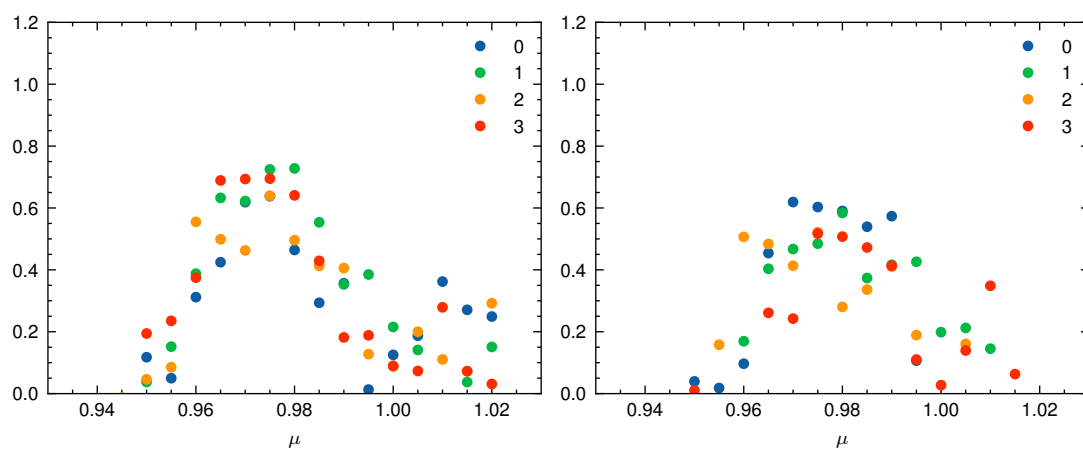


Figure S18: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **6**: Spearman correlation coefficient for IR (left) and Raman (right).

2.6 Compound 7

2.6.1 Alignment Score s and Combined Score

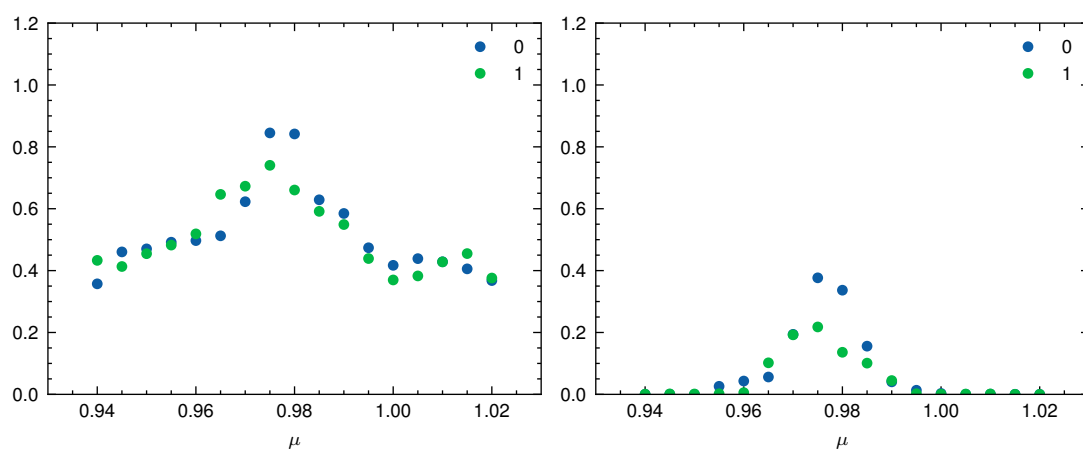


Figure S19: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **7**: total alignment score s (left) and combined score s_{comb} (right).

2.6.2 Pearson Correlation Coefficient

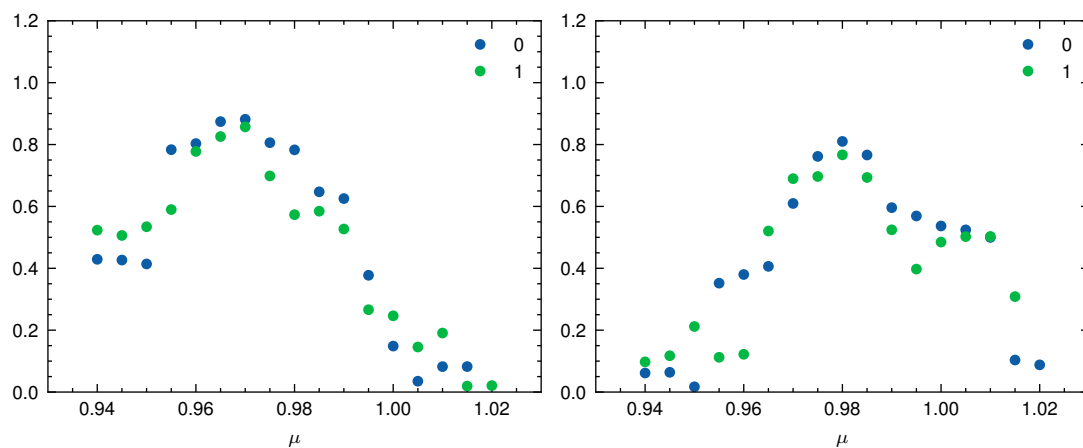


Figure S20: Evaluation metrics as a function of the scaling factor μ for the isomers of compound 7: Pearson correlation coefficient for IR (left) and Raman (right).

2.6.3 Spearman Correlation Coefficient

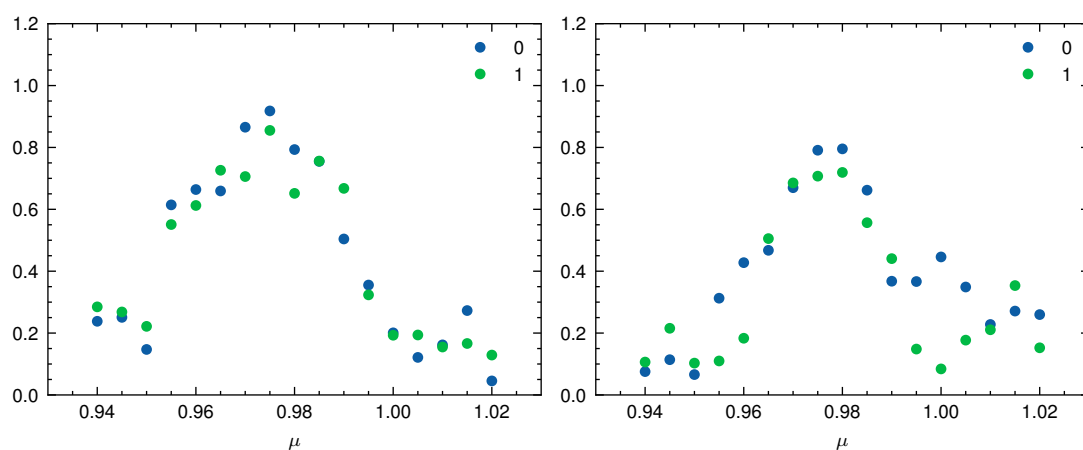


Figure S21: Evaluation metrics as a function of the scaling factor μ for the isomers of compound 7: Spearman correlation coefficient for IR (left) and Raman (right).

2.7 Compound 8

2.7.1 Alignment Score s and Combined Score

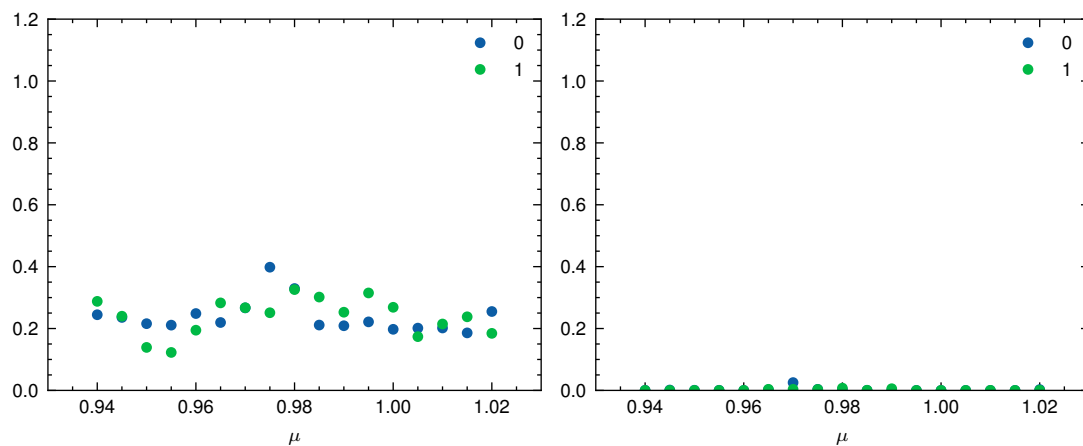


Figure S22: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **2**: total alignment score s (left) and combined score s_{comb} (right).

2.7.2 Pearson Correlation Coefficient

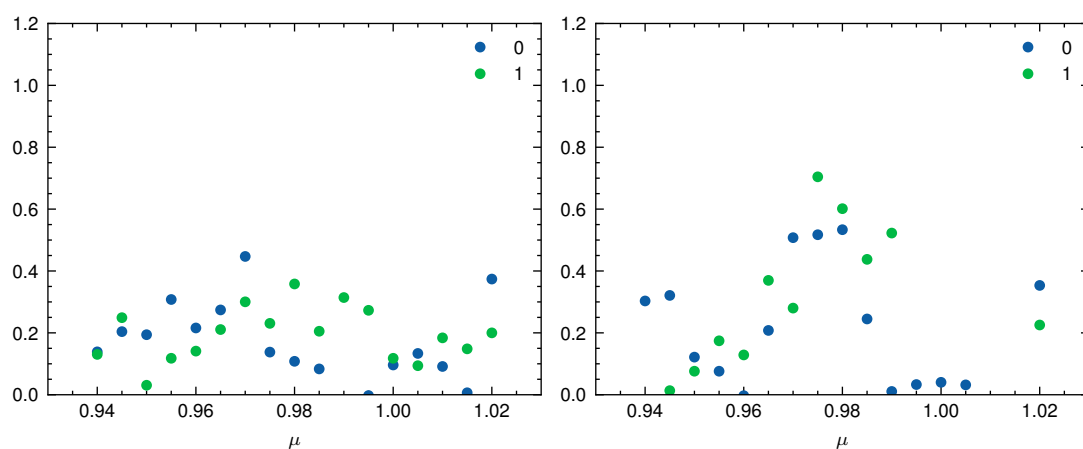


Figure S23: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **8**: Pearson correlation coefficient for IR (left) and Raman (right).

2.7.3 Spearman Correlation Coefficient

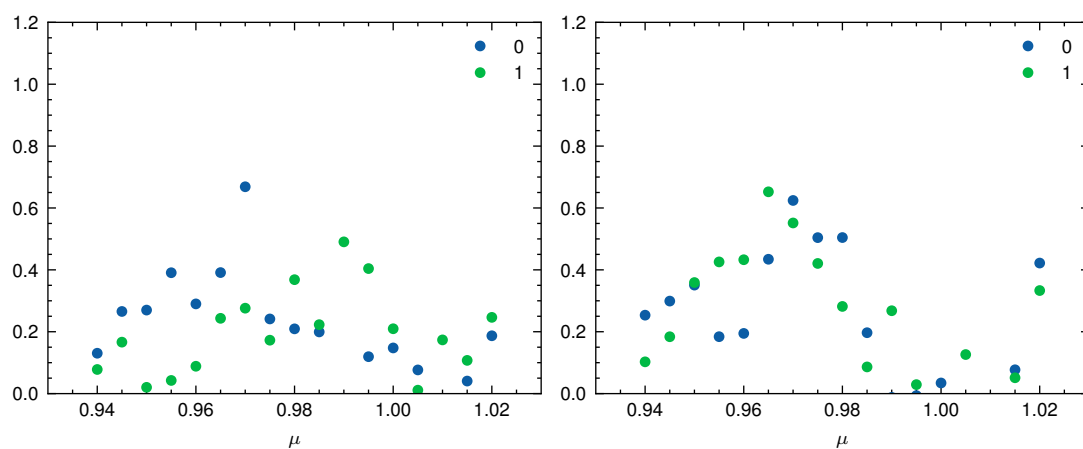


Figure S24: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **8**: Spearman correlation coefficient for IR (left) and Raman (right).

2.8 Compound 9

2.8.1 Alignment Score s and Combined Score

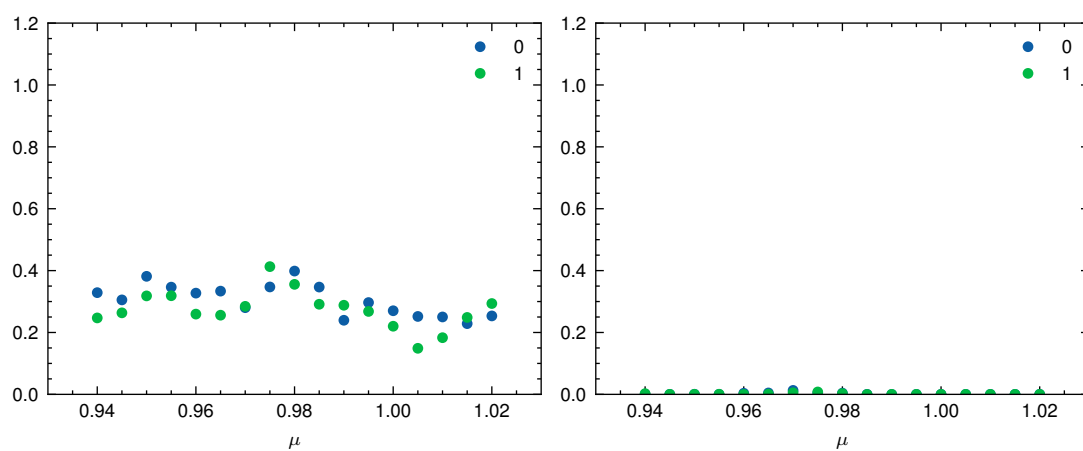


Figure S25: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **9**: total alignment score s (left) and combined score s_{comb} (right).

2.8.2 Pearson Correlation Coefficient

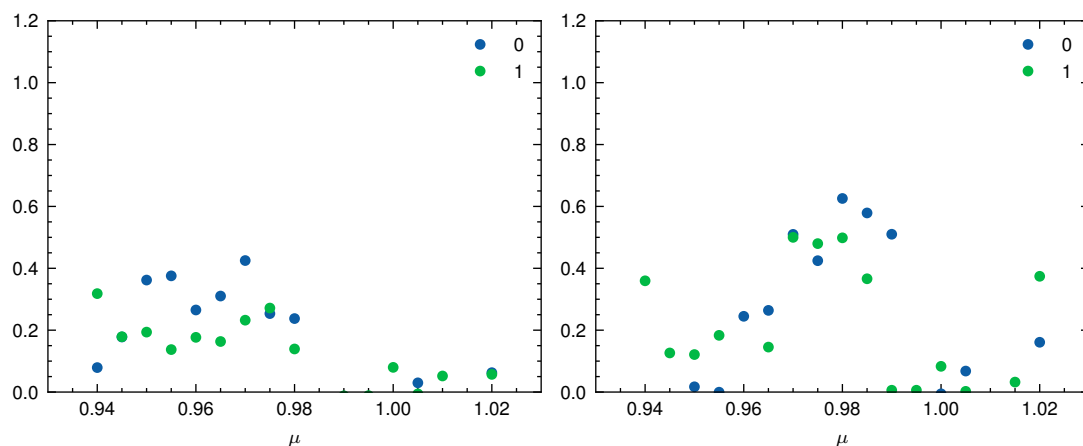


Figure S26: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **9**: Pearson correlation coefficient for IR (left) and Raman (right).

2.8.3 Spearman Correlation Coefficient

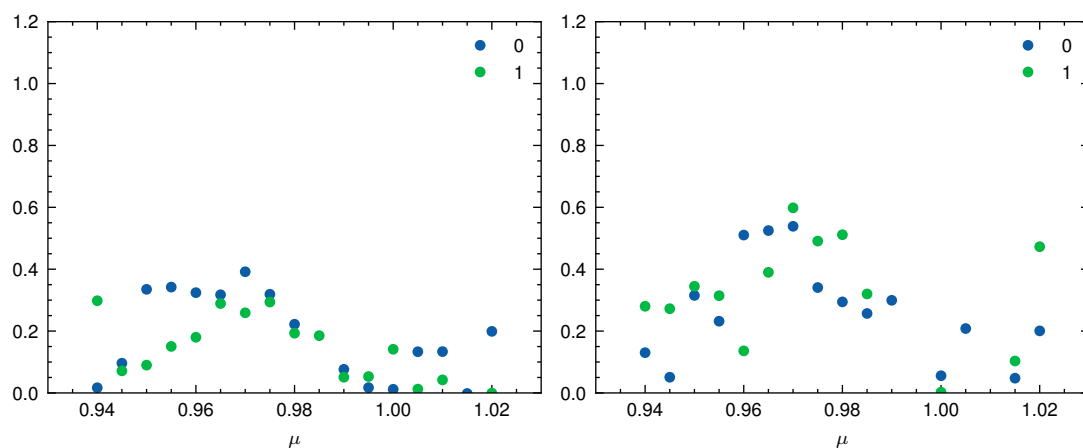


Figure S27: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **9**: Spearman correlation coefficient for IR (left) and Raman (right).

2.9 Compound 10

2.9.1 Alignment Score s and Combined Score

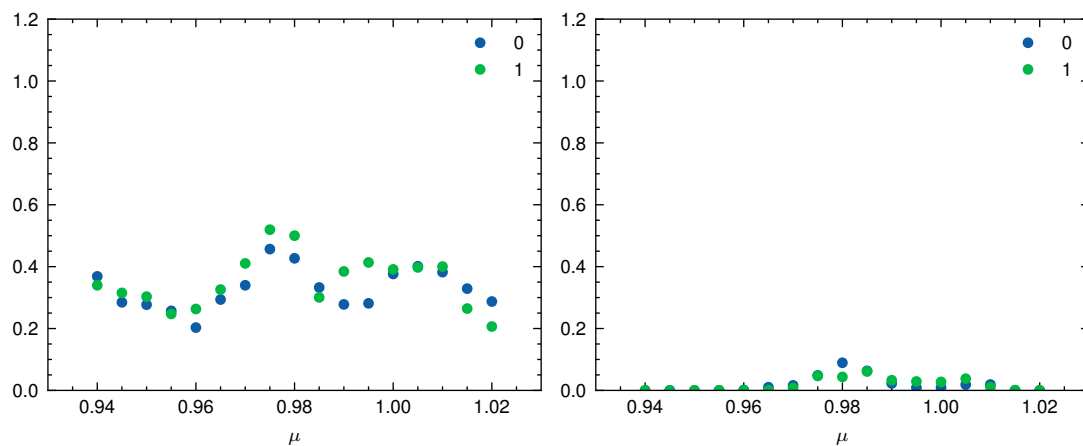


Figure S28: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **10**: total alignment score s (left) and combined score s_{comb} (right).

2.9.2 Pearson Correlation Coefficient

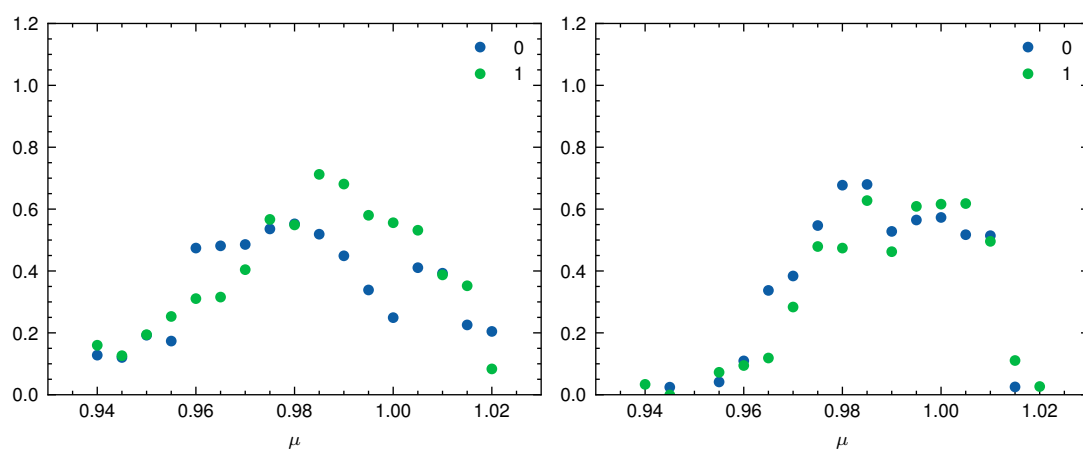


Figure S29: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **10**: Pearson correlation coefficient for IR (left) and Raman (right).

2.9.3 Spearman Correlation Coefficient

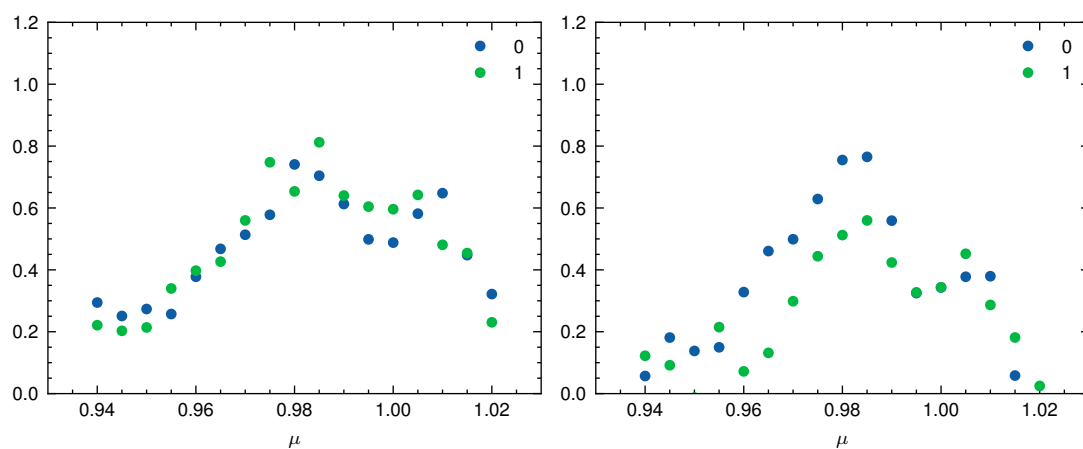


Figure S30: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **10**: Spearman correlation coefficient for IR (left) and Raman (right).

2.10 Compound 11

2.10.1 Alignment Score s and Combined Score

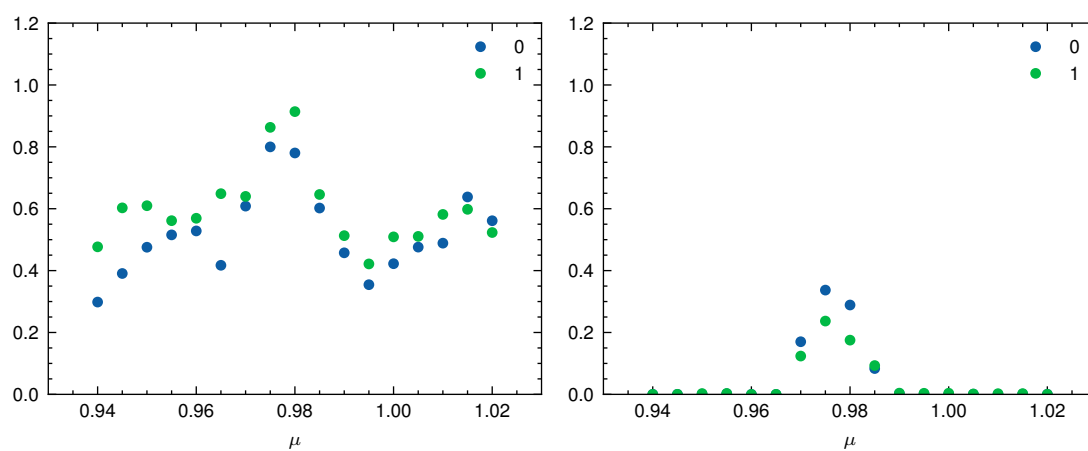


Figure S31: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **11**: total alignment score s (left) and combined score s_{comb} (right).

2.10.2 Pearson Correlation Coefficient

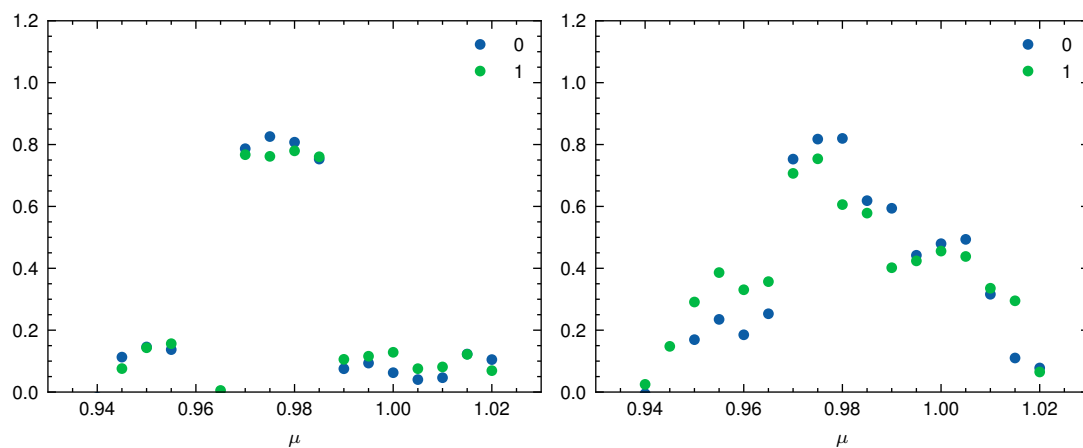


Figure S32: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **11**: Pearson correlation coefficient for IR (left) and Raman (right).

2.10.3 Spearman Correlation Coefficient

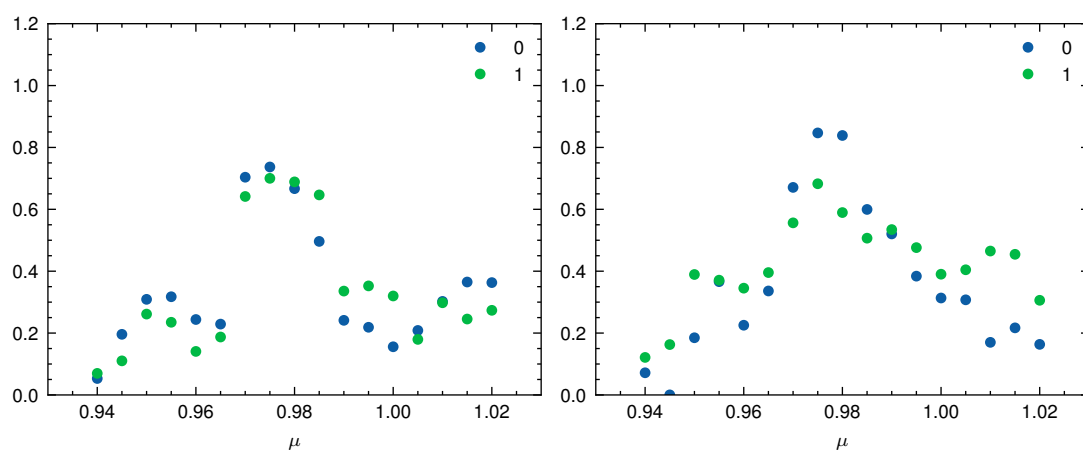


Figure S33: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **11**: Spearman correlation coefficient for IR (left) and Raman (right).

2.11 Compound 12

2.11.1 Alignment Score s and Combined Score

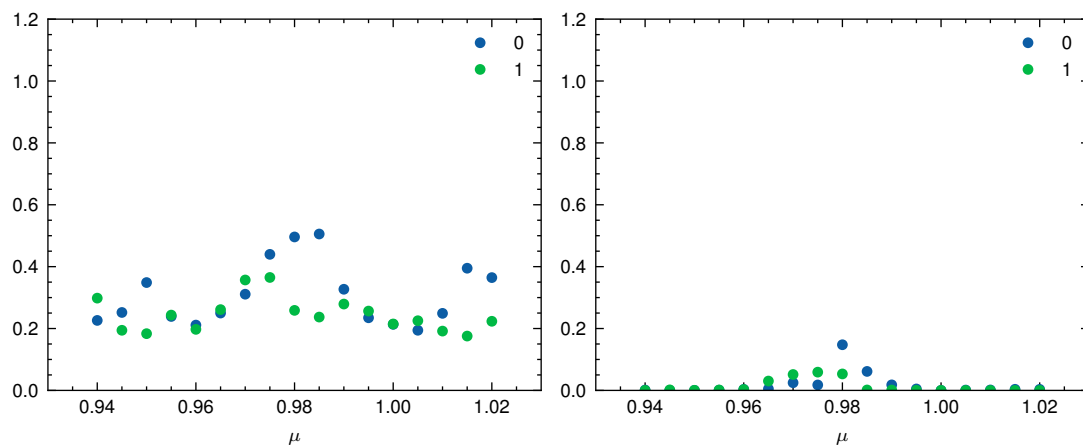


Figure S34: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **12**: total alignment score s (left) and combined score s_{comb} (right).

2.11.2 Pearson Correlation Coefficient

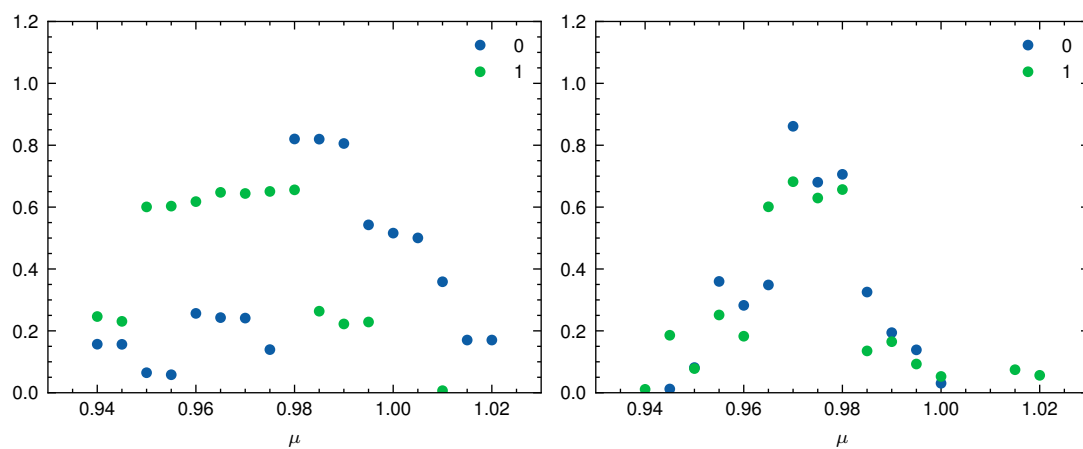


Figure S35: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **12**: Pearson correlation coefficient for IR (left) and Raman (right).

2.11.3 Spearman Correlation Coefficient

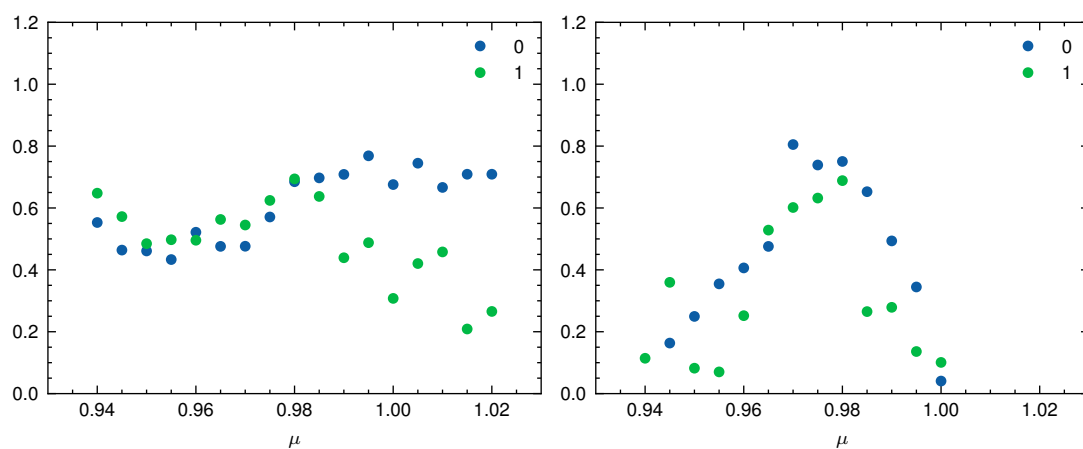


Figure S36: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **12**: Spearman correlation coefficient for IR (left) and Raman (right).

2.12 Compound 13

2.12.1 Alignment Score s and Combined Score

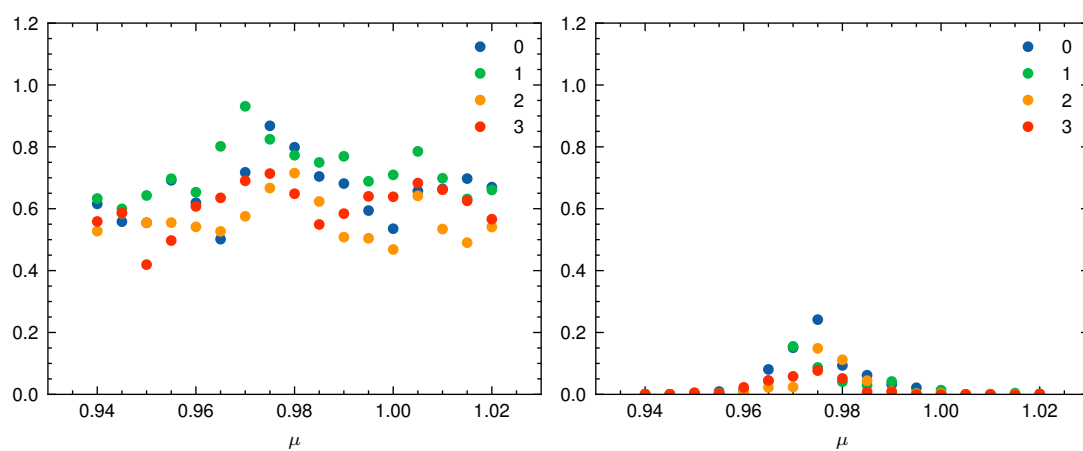


Figure S37: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **13**: total alignment score s (left) and combined score s_{comb} (right).

2.12.2 Pearson Correlation Coefficient

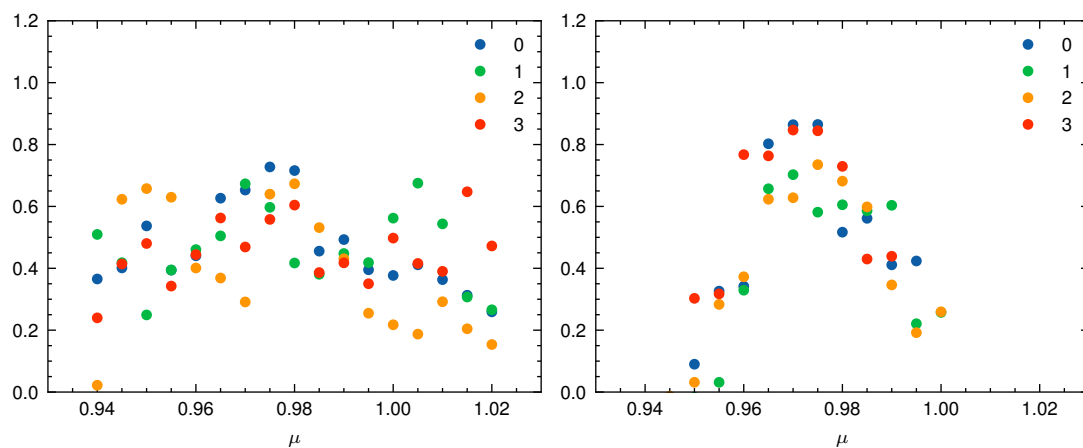


Figure S38: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **13**: Pearson correlation coefficient for IR (left) and Raman (right).

2.12.3 Spearman Correlation Coefficient

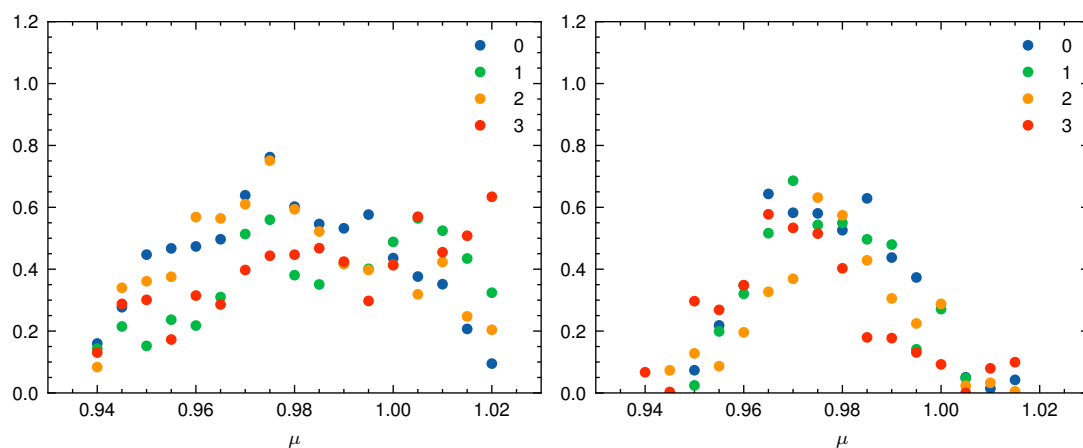


Figure S39: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **13**: Spearman correlation coefficient for IR (left) and Raman (right).

2.13 Compound 14

2.13.1 Alignment Score s and Combined Score

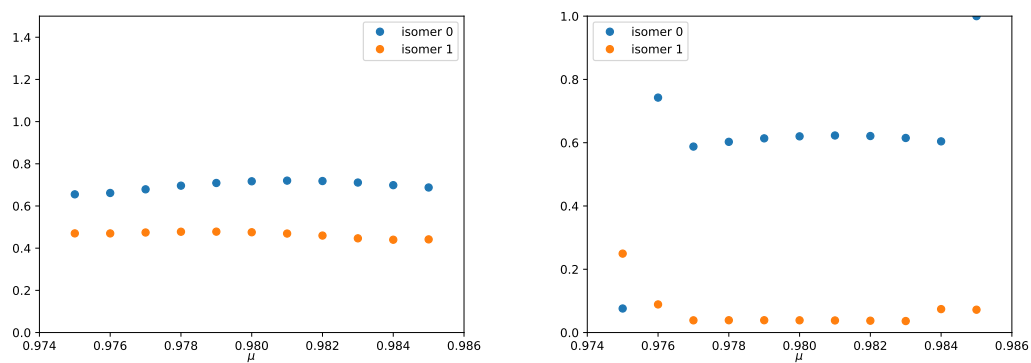


Figure S40: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **14**: total alignment score s (left) and combined score s_{comb} (right).

2.13.2 Pearson Correlation Coefficient

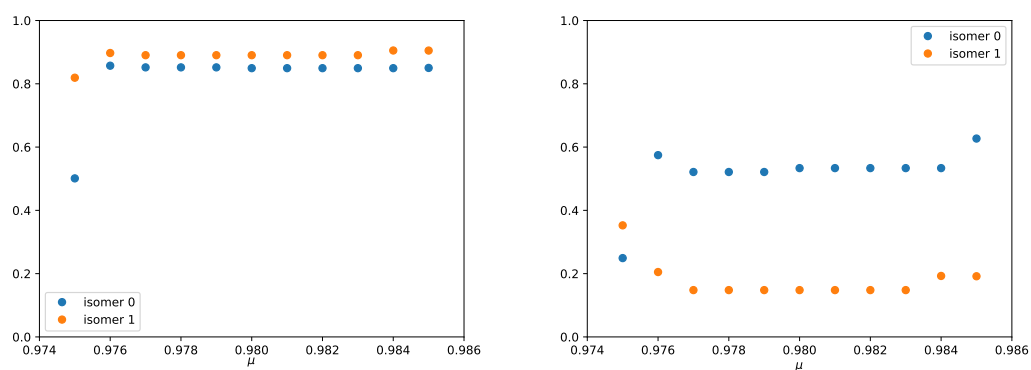


Figure S41: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **14**: Pearson correlation coefficient for IR (left) and Raman (right).

2.13.3 Spearman Correlation Coefficient

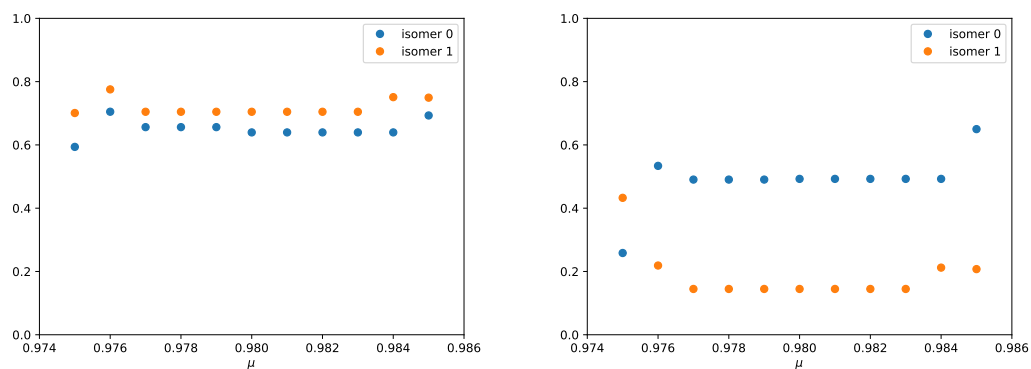


Figure S42: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **14**: Spearman correlation coefficient for IR (left) and Raman (right).

2.14 VCD spectra

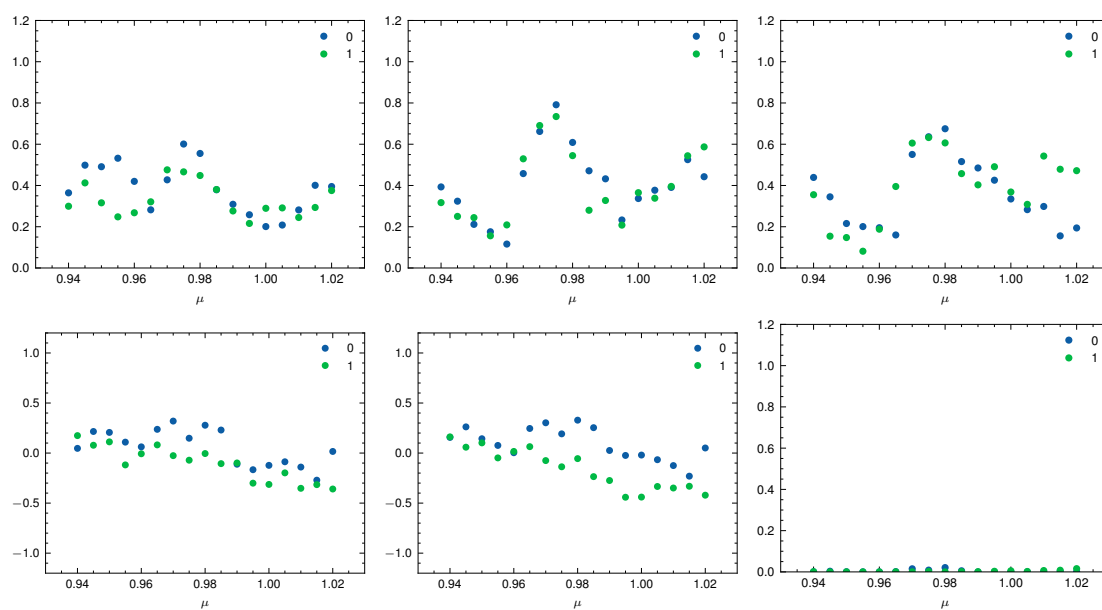


Figure S43: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **15**: total alignment score s (top left), combined score s_{comb} (bottom right), Pearson and Spearman correlation coefficients (remaining panels) for the IR and VCD spectra.

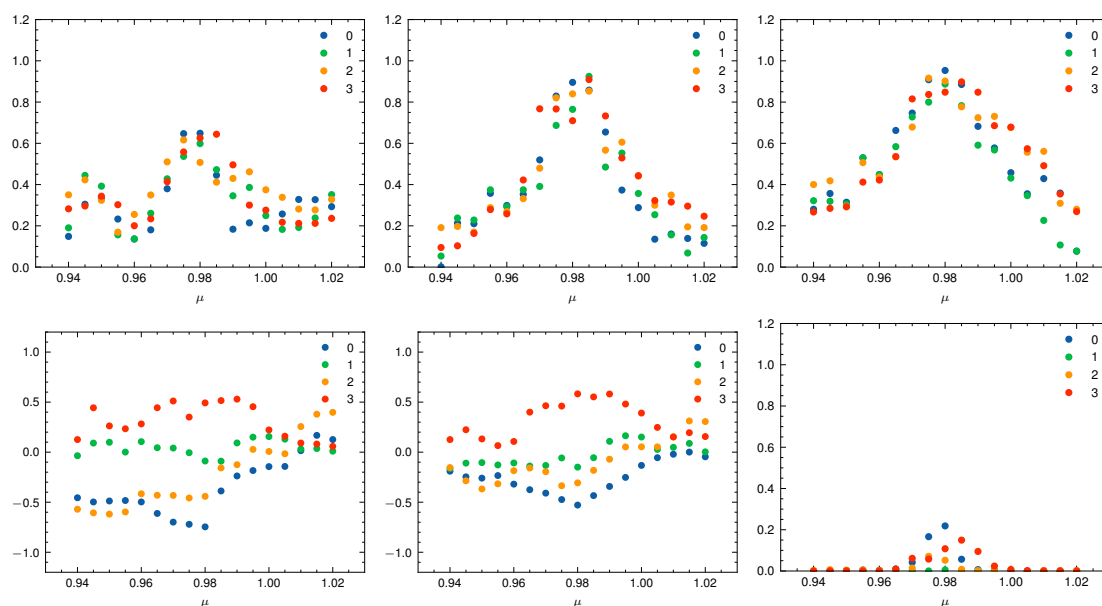


Figure S44: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **16**: total alignment score s (top left), combined score s_{comb} (bottom right), Pearson and Spearman correlation coefficients (remaining panels) for the IR and VCD spectra.

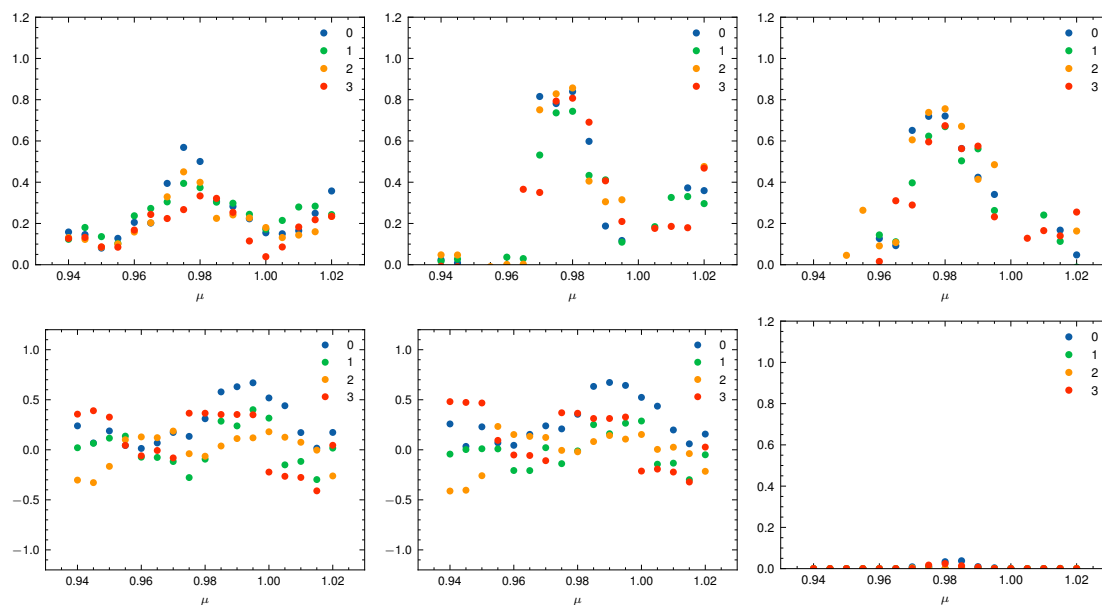


Figure S45: Evaluation metrics as a function of the scaling factor μ for the isomers of compound **17**: total alignment score s (top left), combined score s_{comb} (bottom right), Pearson and Spearman correlation coefficients (remaining panels) for the IR and VCD spectra.

3 Aligned Spectra

All presented results employ $\mu = 0.98$.

3.1 Compound 1

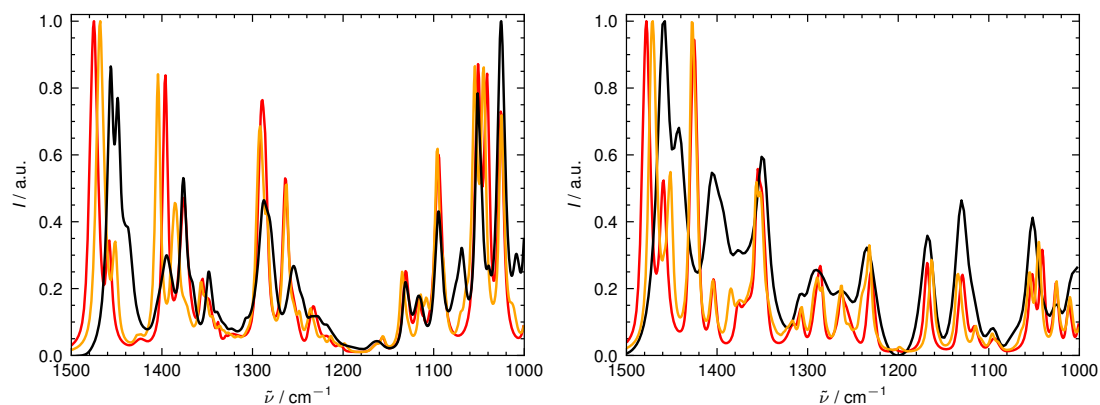


Figure S46: Aligned spectrum of compound **1**, isomer 0. Left: IR, Right: Raman.

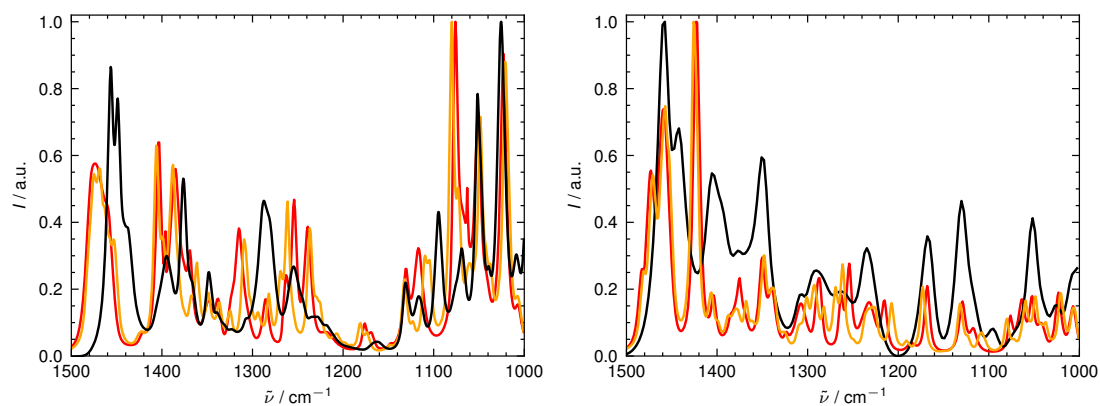


Figure S47: Aligned spectrum of compound **1** isomer 1. Left: IR, Right: Raman.

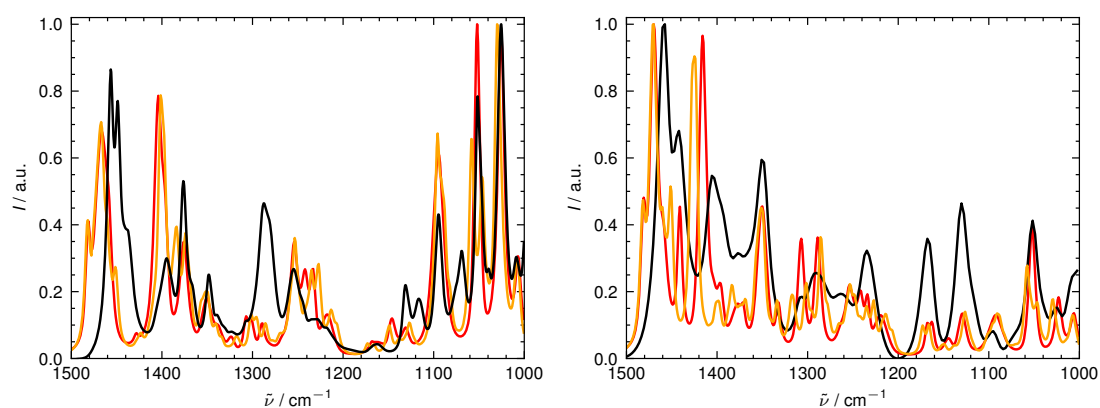


Figure S48: Aligned spectrum of compound **1**, isomer 2. Left: IR, Right: Raman.

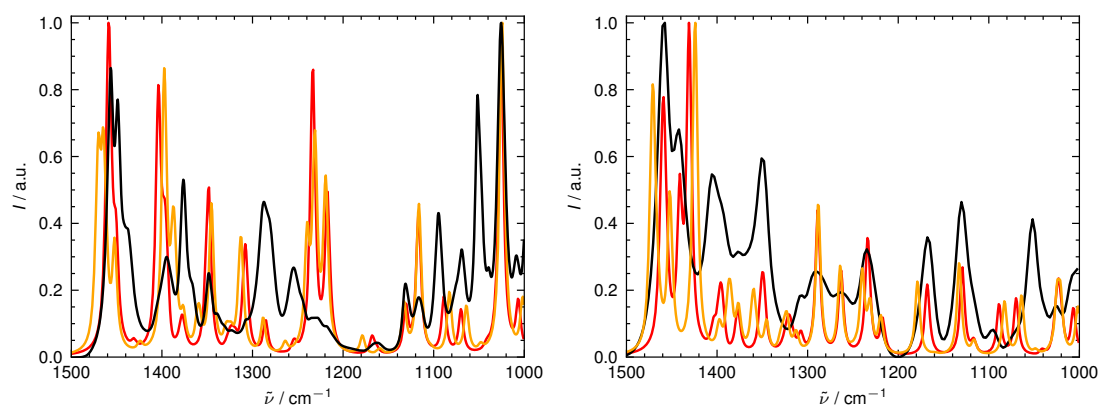


Figure S49: Aligned spectrum of compound **1**, isomer 3. Left: IR, Right: Raman.

3.2 Compound 2

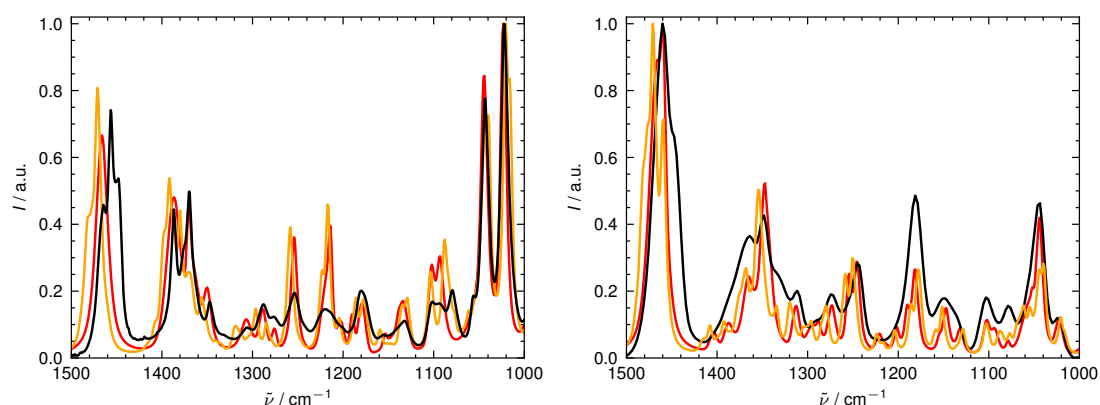


Figure S50: Aligned spectrum of compound **2**, isomer 0. Left: IR, Right: Raman.

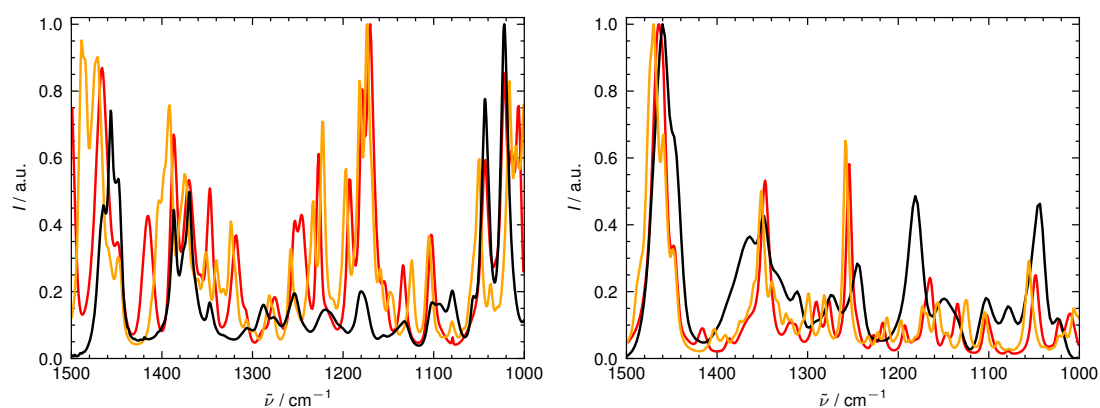


Figure S51: Aligned spectrum of compound **2**, isomer 1. Left: IR, Right: Raman.

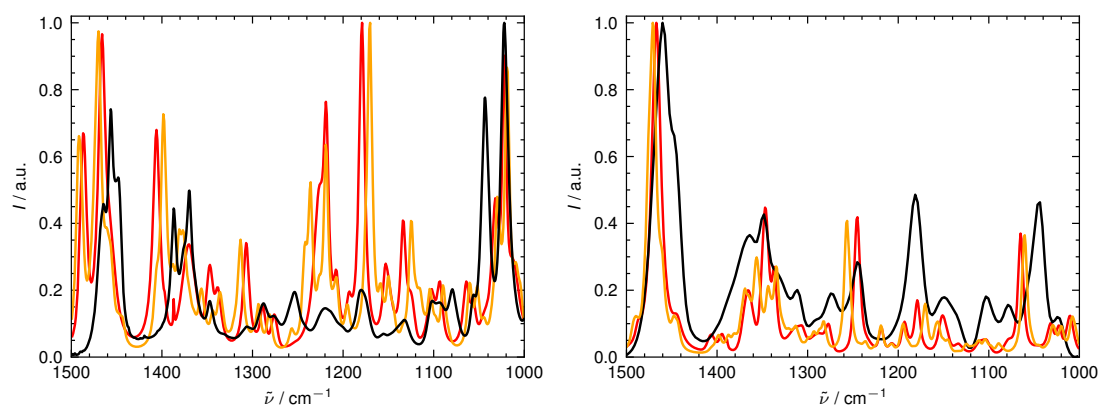


Figure S52: Aligned spectrum of compound **2**, isomer 2. Left: IR, Right: Raman.

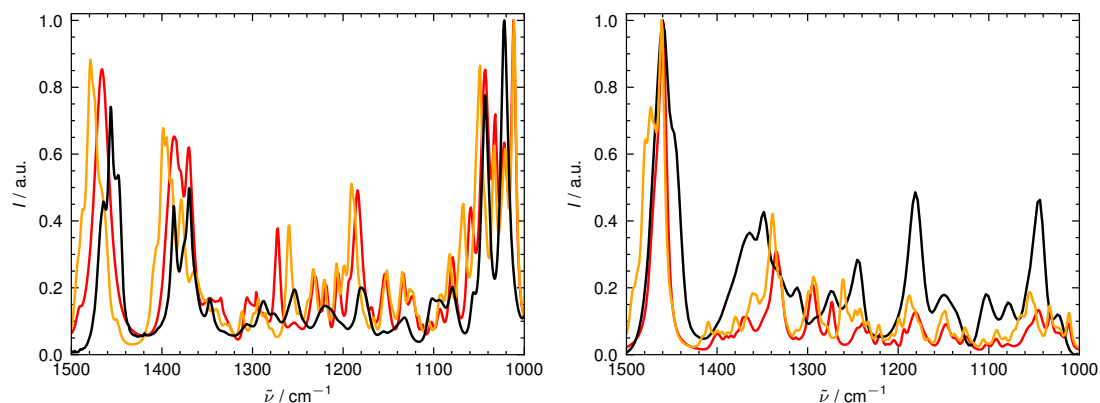


Figure S53: Aligned spectrum of compound **2**, isomer 3. Left: IR, Right: Raman.

3.3 Compound 3

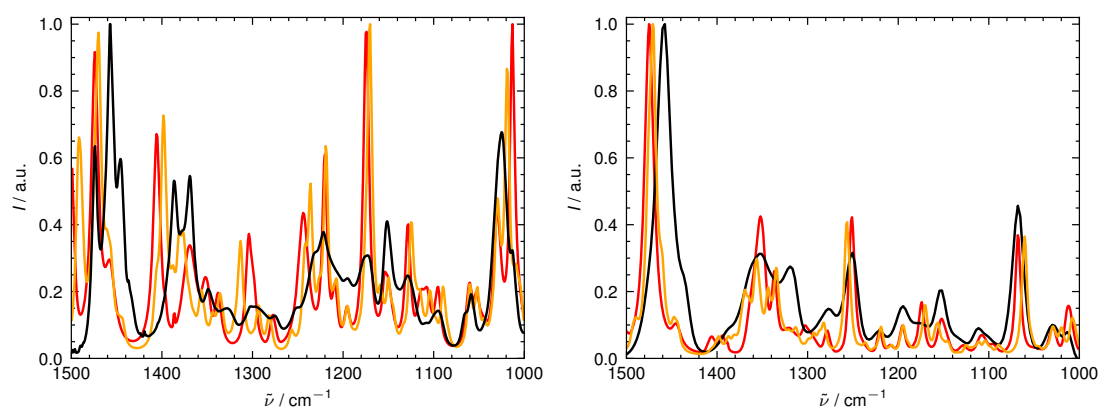


Figure S54: Aligned spectrum of compound **3**, isomer 0. Left: IR, Right: Raman.

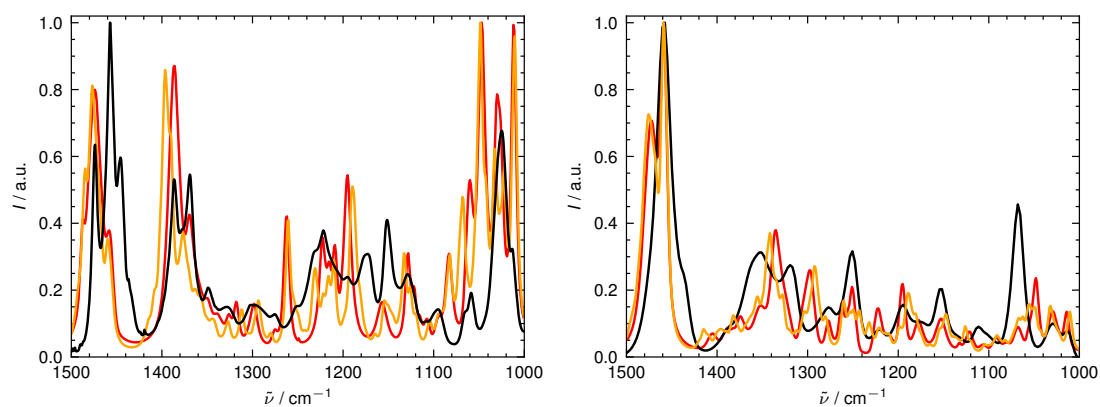


Figure S55: Aligned spectrum of compound **3**, isomer 1. Left: IR, Right: Raman.

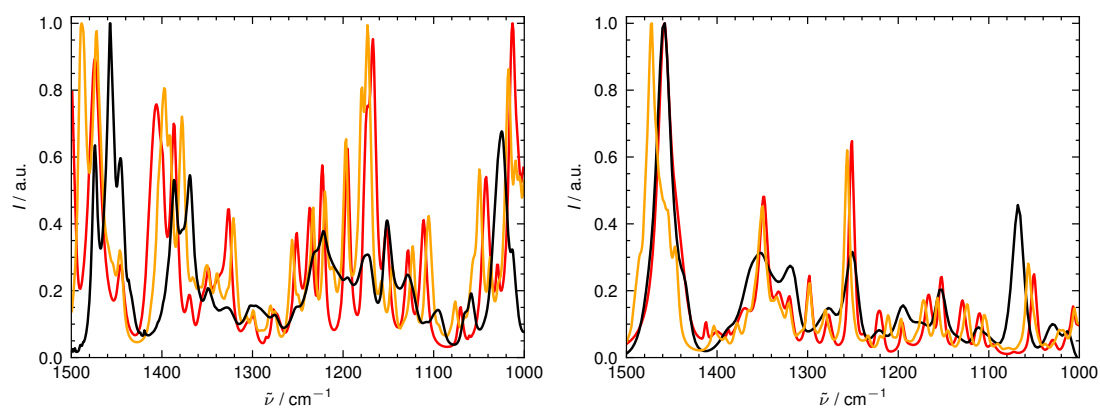


Figure S56: Aligned spectrum of compound **3**, isomer 2. Left: IR, Right: Raman.

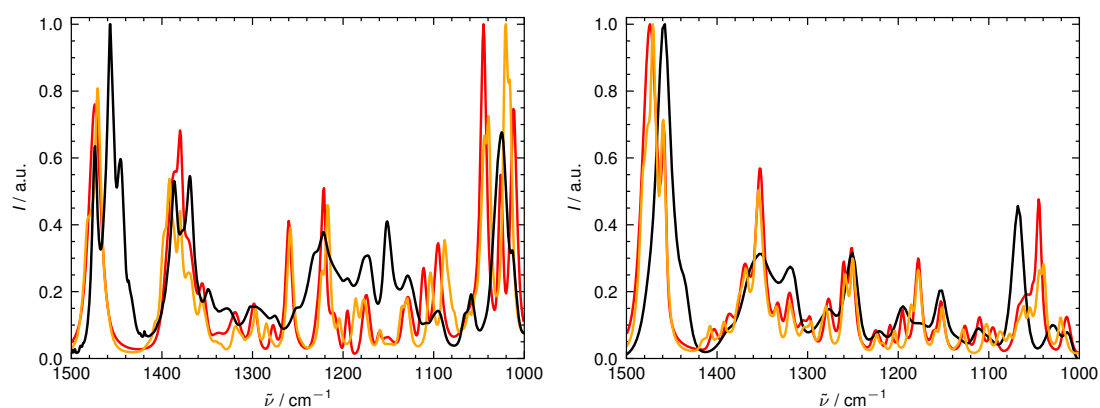


Figure S57: Aligned spectrum of compound **3**, isomer 3. Left: IR, Right: Raman.

3.4 Compound 4

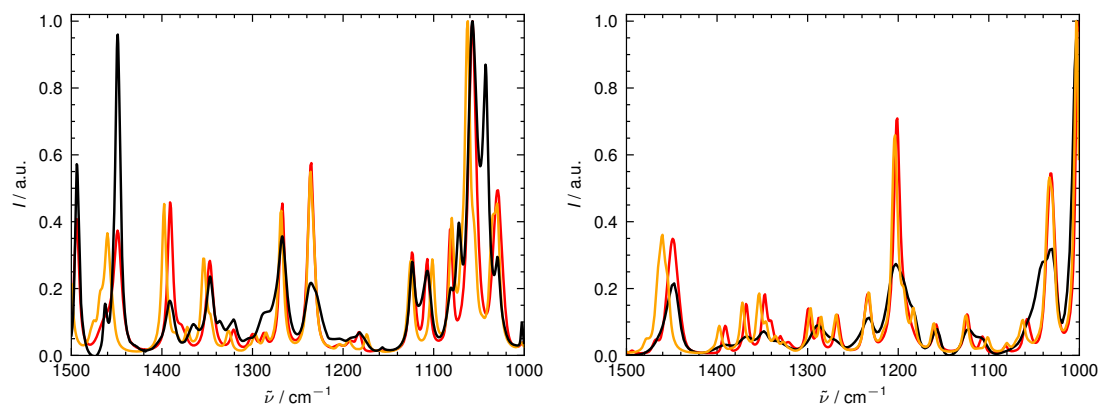


Figure S58: Aligned spectrum of compound **4**, isomer 0. Left: IR, Right: Raman.

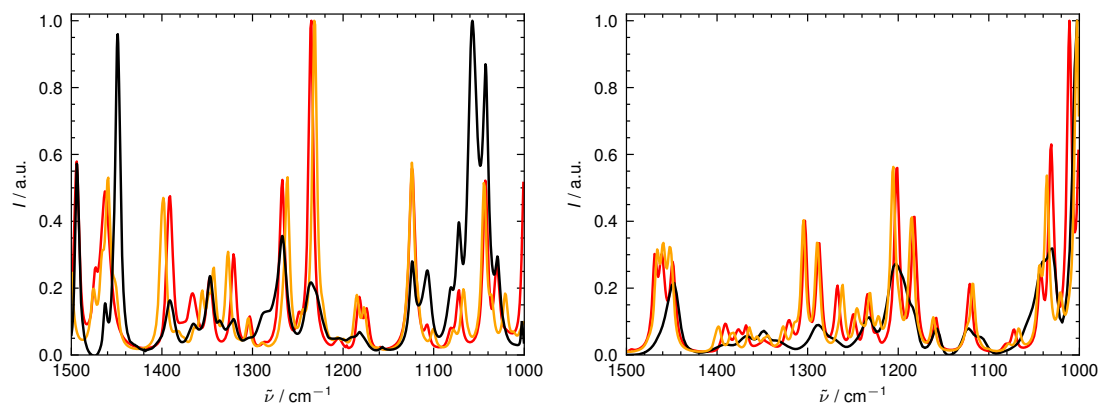


Figure S59: Aligned spectrum of compound **4**, isomer 1. Left: IR, Right: Raman.

3.5 Compound 5

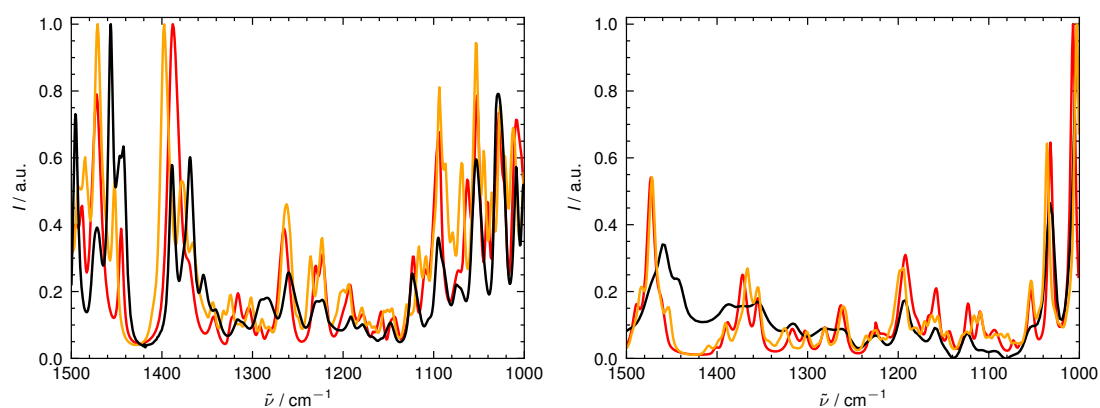


Figure S60: Aligned spectrum of compound **5**, isomer 0. Left: IR, Right: Raman.

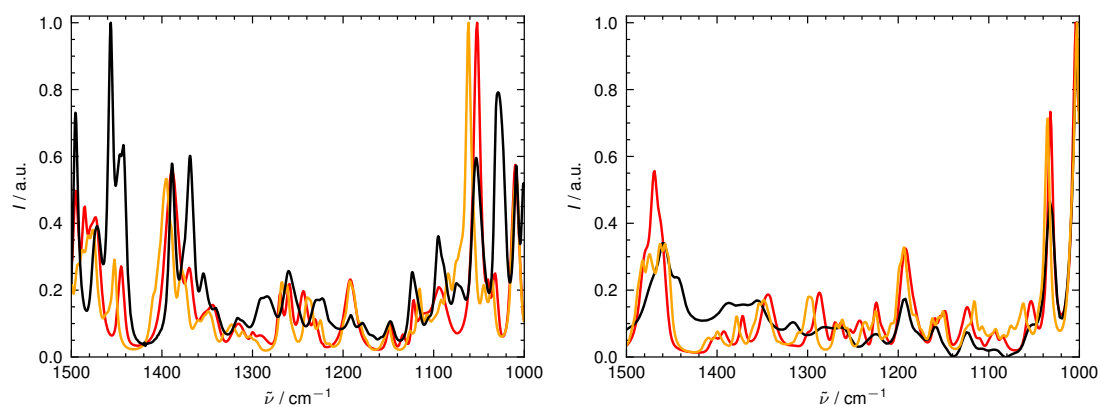


Figure S61: Aligned spectrum of compound **5**, isomer 1. Left: IR, Right: Raman.

3.6 Compound 6

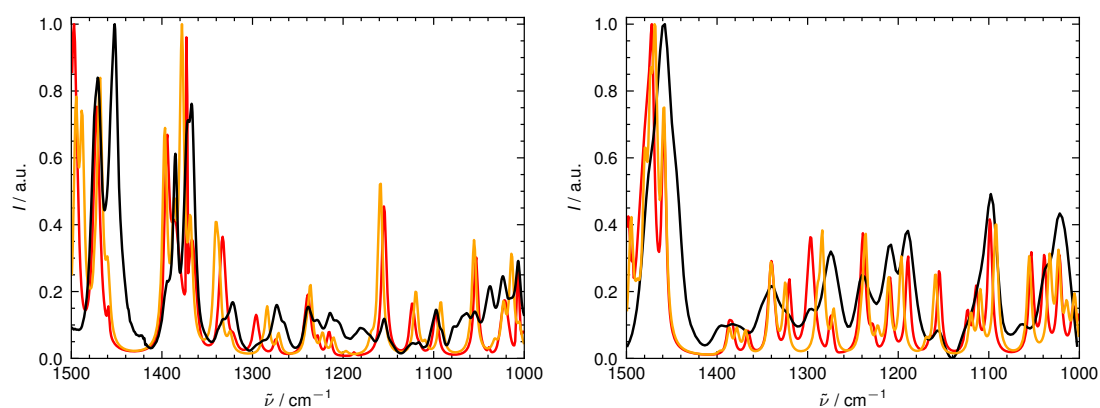


Figure S62: Aligned spectrum of compound **6**, isomer 0. Left: IR, Right: Raman.

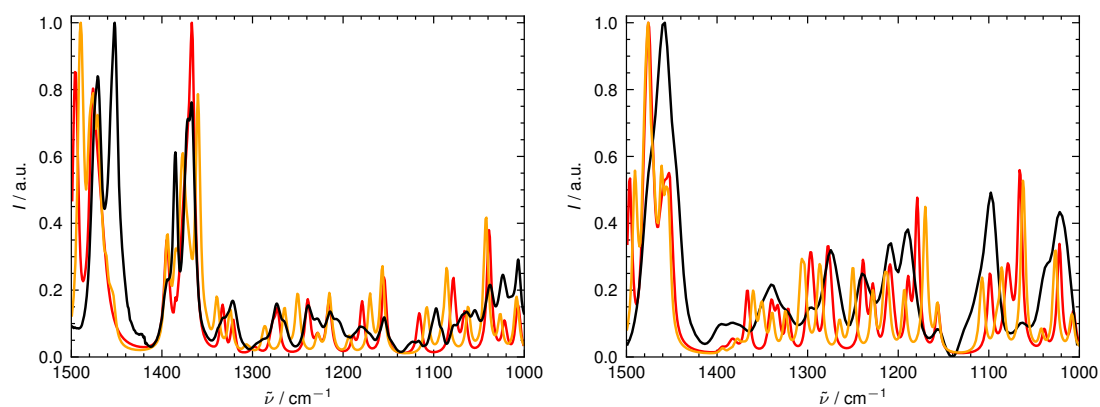


Figure S63: Aligned spectrum of compound **6**, isomer 1. Left: IR, Right: Raman.

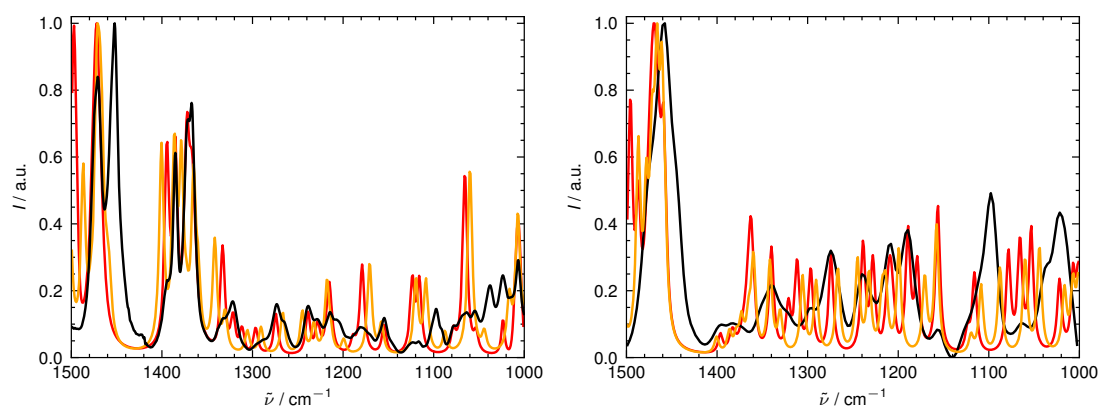


Figure S64: Aligned spectrum of compound **6**, isomer 2. Left: IR, Right: Raman.

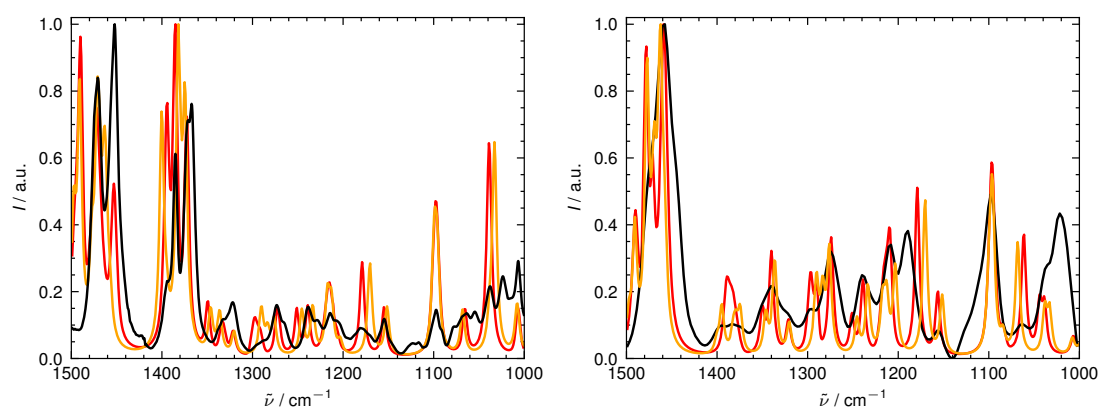


Figure S65: Aligned spectrum of compound **6**, isomer 3. Left: IR, Right: Raman.

3.7 Compound 7

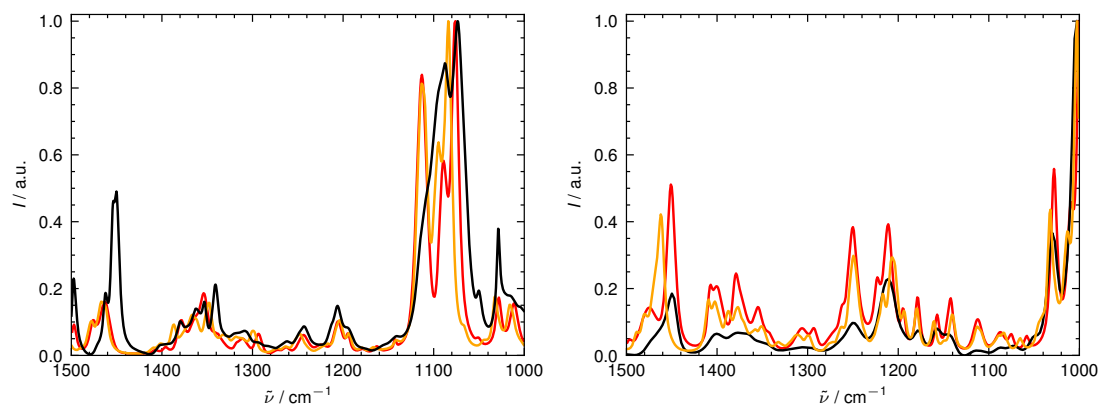


Figure S66: Aligned spectrum of compound **7**, isomer 0. Left: IR, Right: Raman.

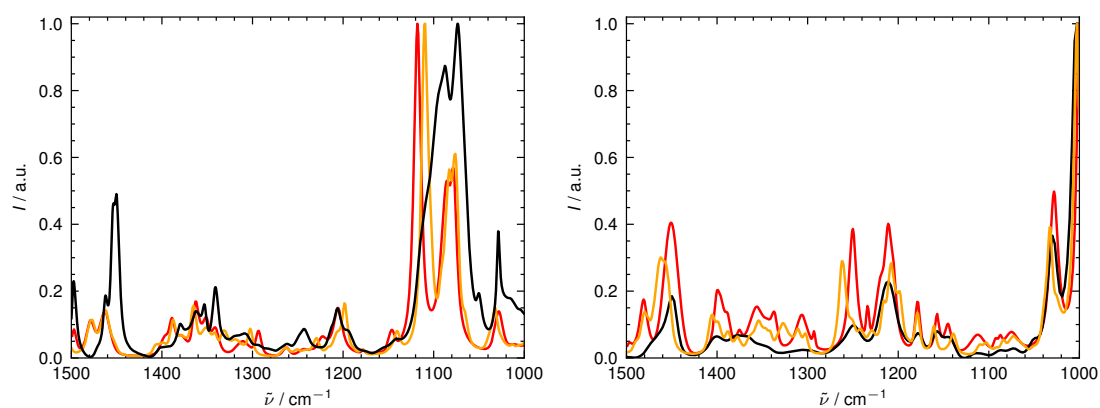


Figure S67: Aligned spectrum of compound **7**, isomer 1. Left: IR, Right: Raman.

3.8 Compound 8

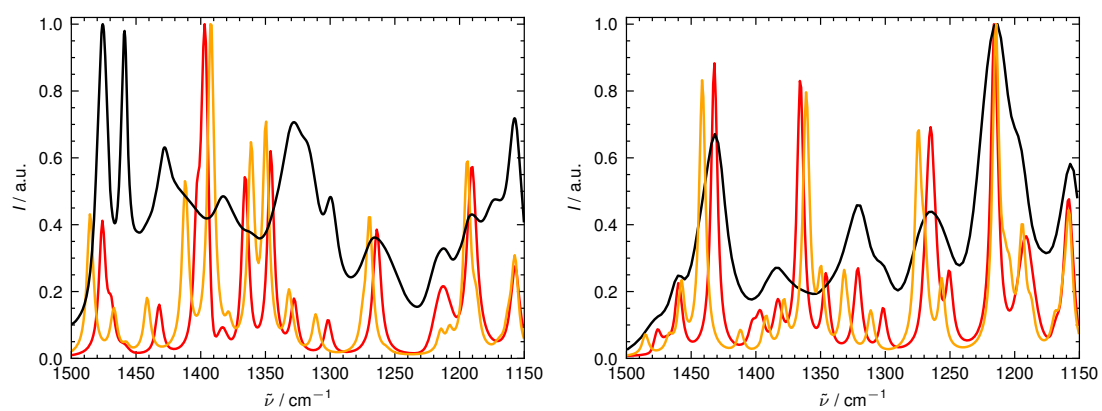


Figure S68: Aligned spectrum of compound **8**, isomer 0. Left: IR, Right: Raman.

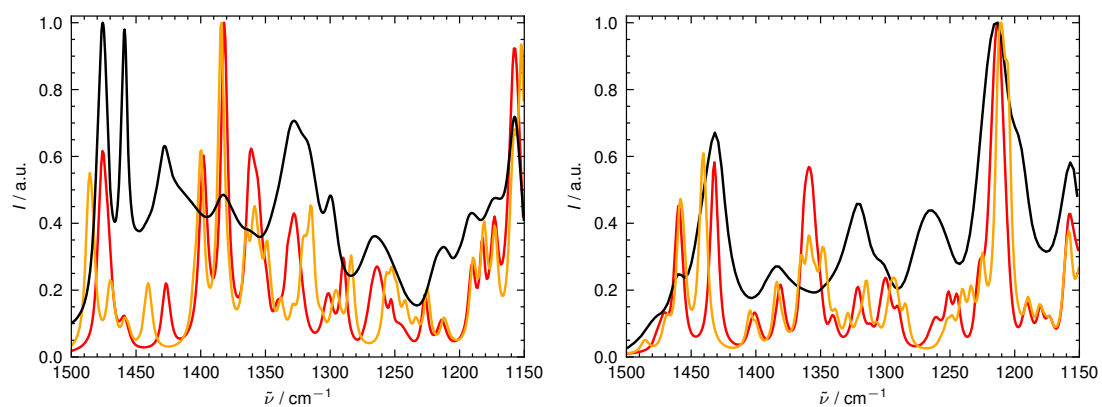


Figure S69: Aligned spectrum of compound **8**, isomer 1. Left: IR, Right: Raman.

3.9 Compound 9

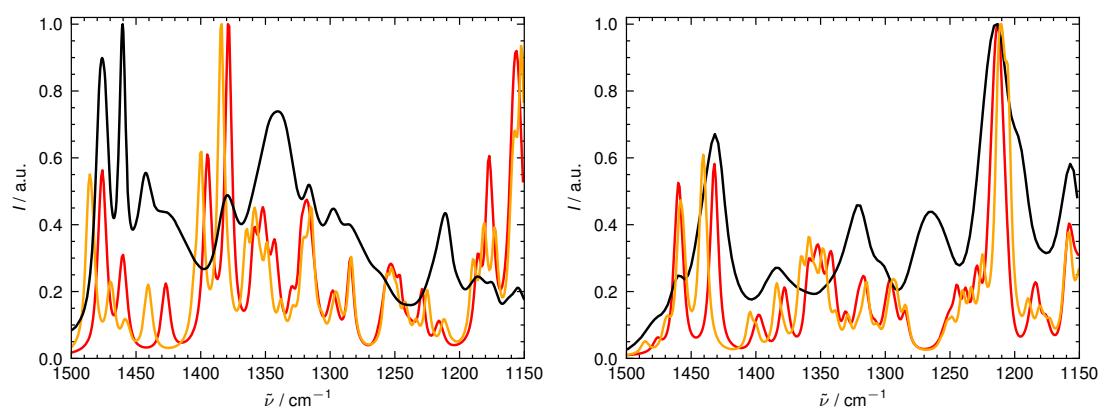


Figure S70: Aligned spectrum of compound **9**, isomer 0. Left: IR, Right: Raman.

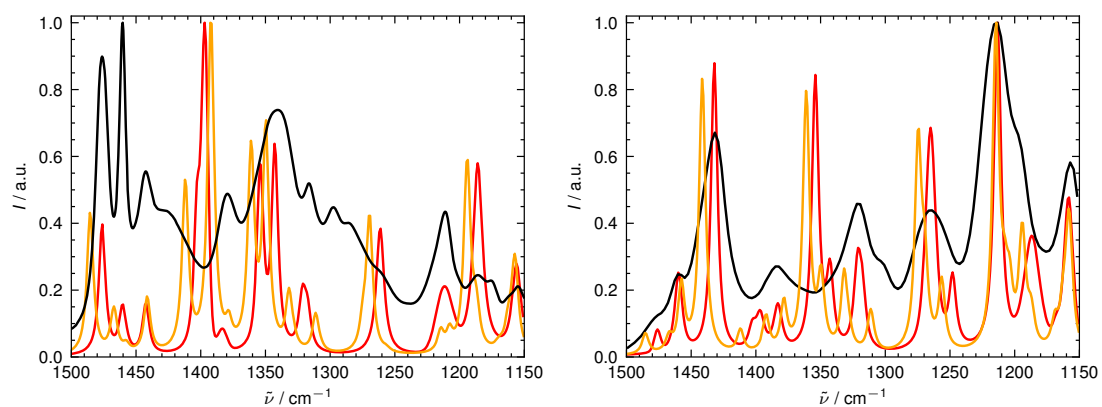


Figure S71: Aligned spectrum of compound **9**, isomer 1. Left: IR, Right: Raman.

3.10 Compound 10

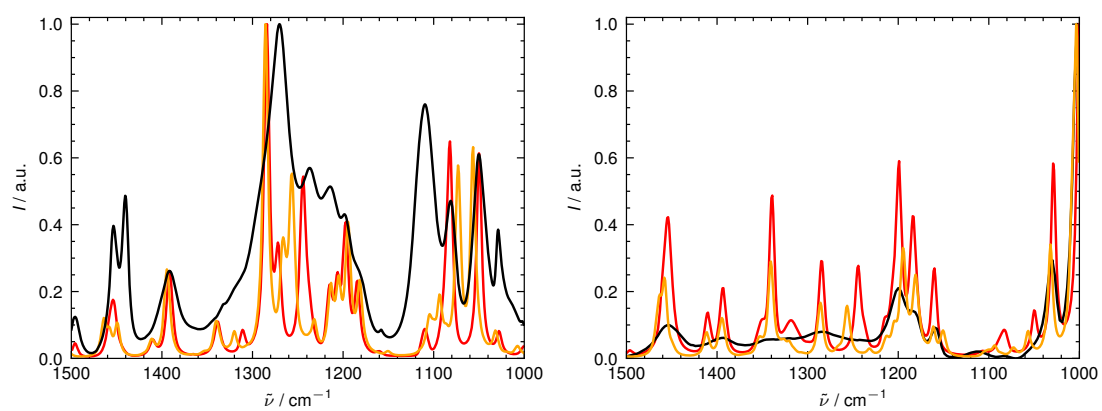


Figure S72: Aligned spectrum of compound **10**, isomer 0. Left: IR, Right: Raman.

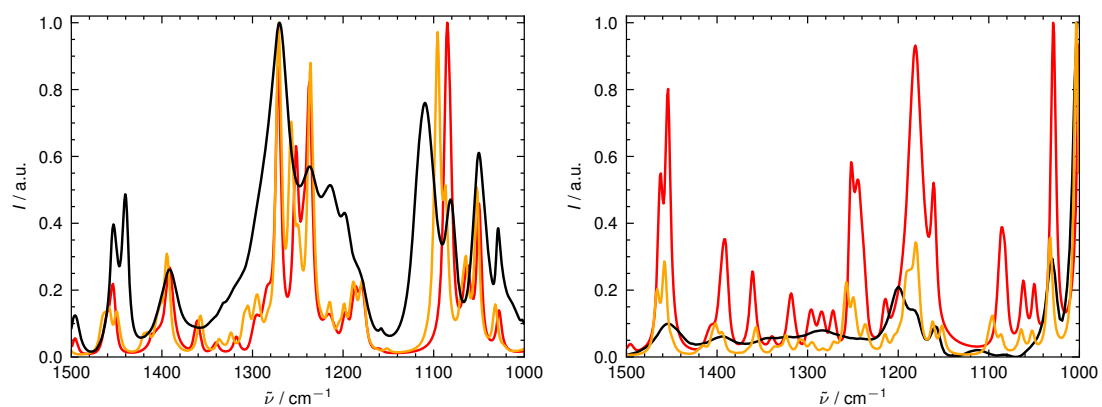


Figure S73: Aligned spectrum of compound **9**, isomer 1. Left: IR, Right: Raman.

3.11 Compound 11

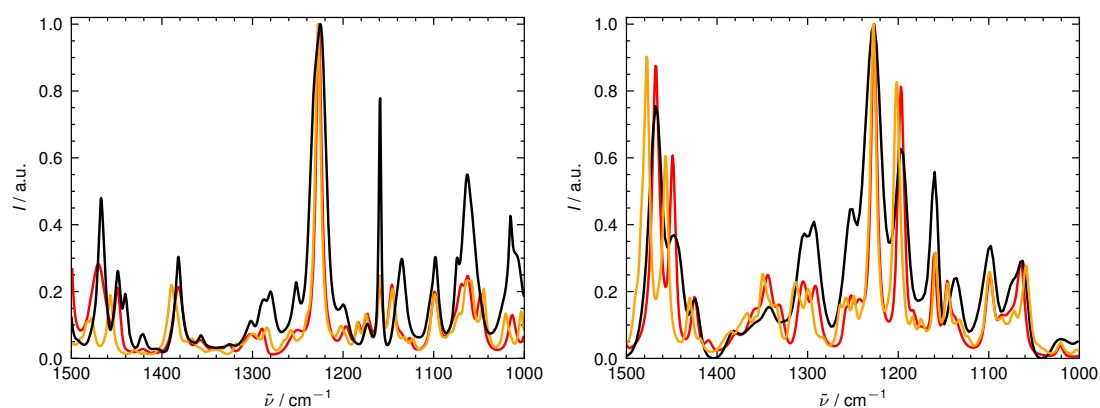


Figure S74: Aligned spectrum of compound 11, isomer 0. Left: IR, Right: Raman.

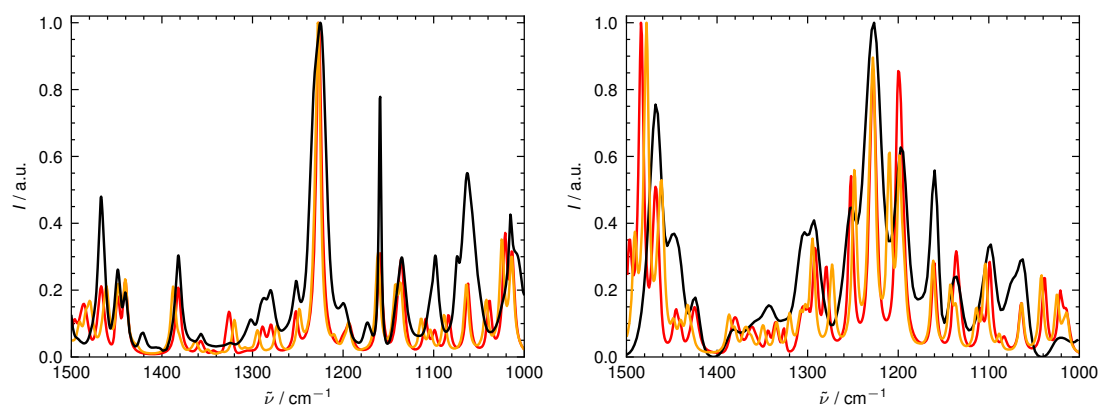


Figure S75: Aligned spectrum of compound 11, isomer 1. Left: IR, Right: Raman.

3.12 Compound 12

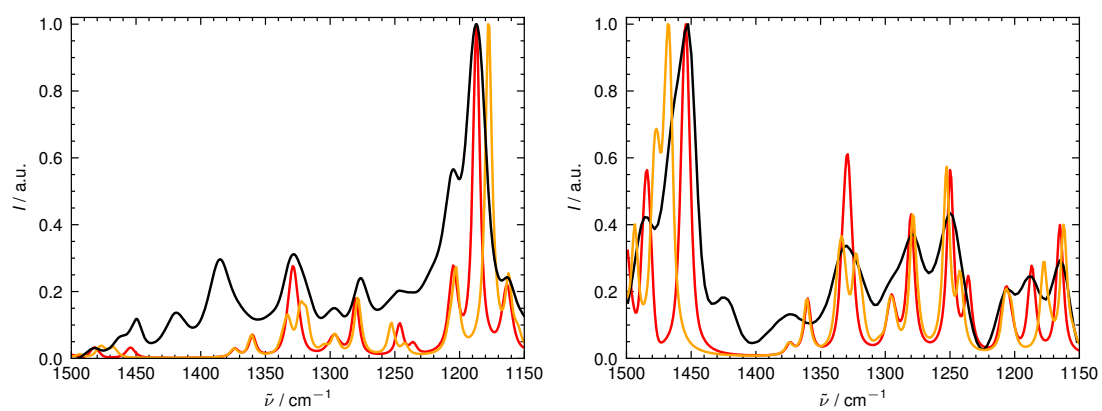


Figure S76: Aligned spectrum of compound 12, isomer 0. Left: IR, Right: Raman.

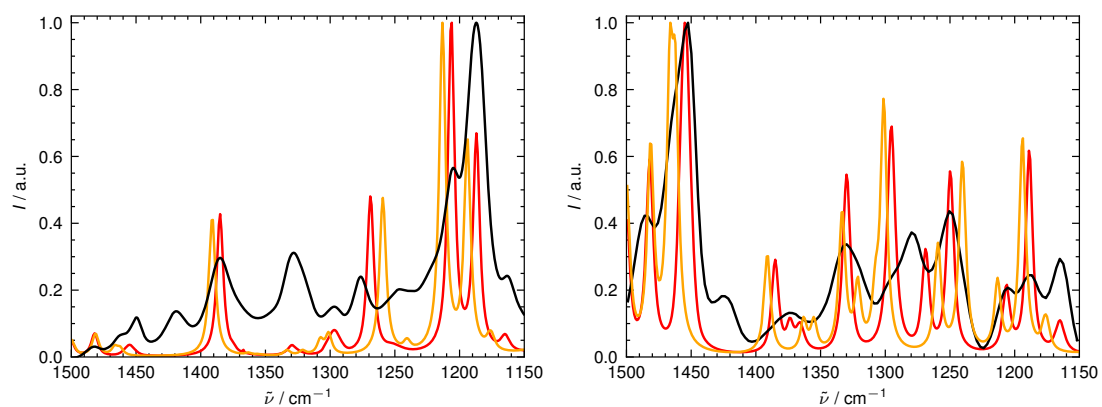


Figure S77: Aligned spectrum of compound 12, isomer 1. Left: IR, Right: Raman.

3.13 Compound 13

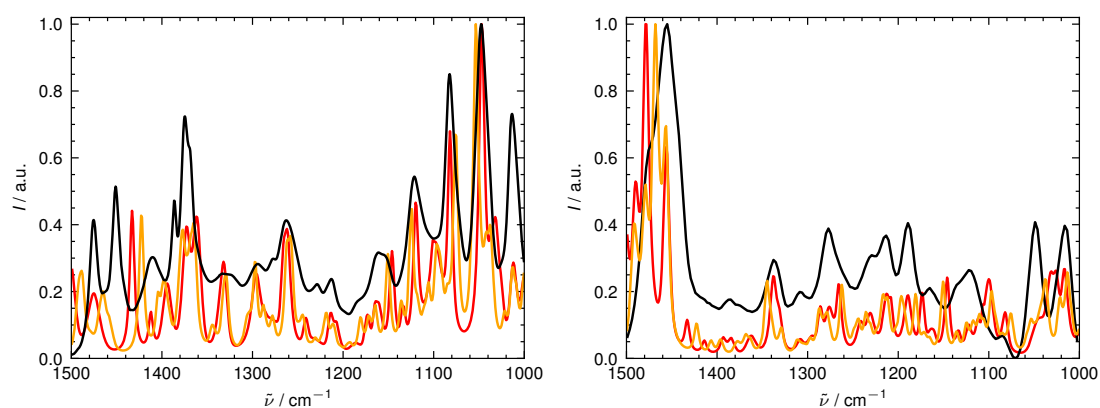


Figure S78: Aligned spectrum of compound **13**, isomer 0. Left: IR, Right: Raman.

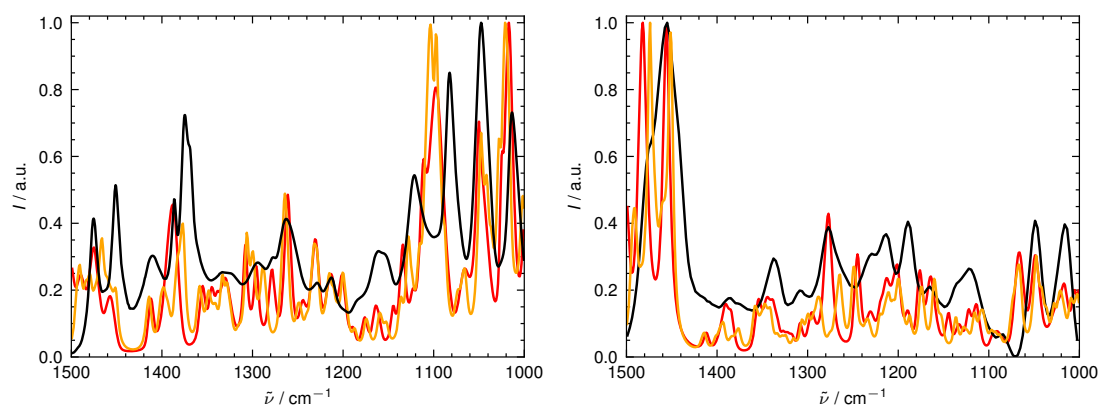


Figure S79: Aligned spectrum of compound **13**, isomer 1. Left: IR, Right: Raman.

3.14 Compound 14

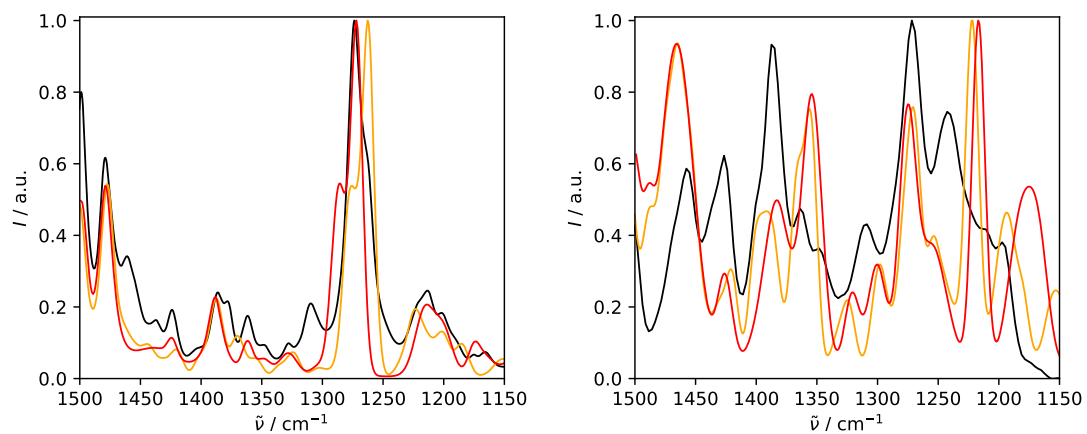


Figure S80: Aligned spectrum of compound **14**, isomer 0. Left: IR, Right: Raman.

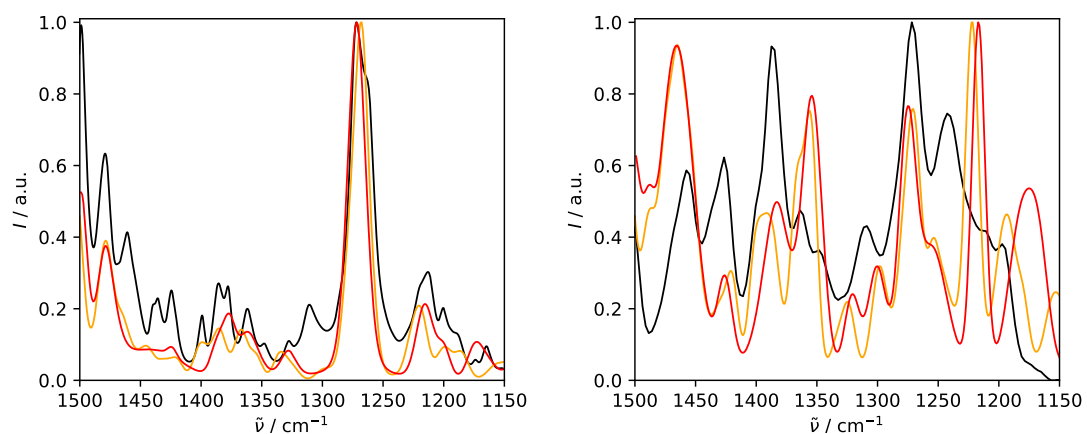


Figure S81: Aligned spectrum of compound **14**, isomer 1. Left: IR, Right: Raman.

3.15 Compound 15

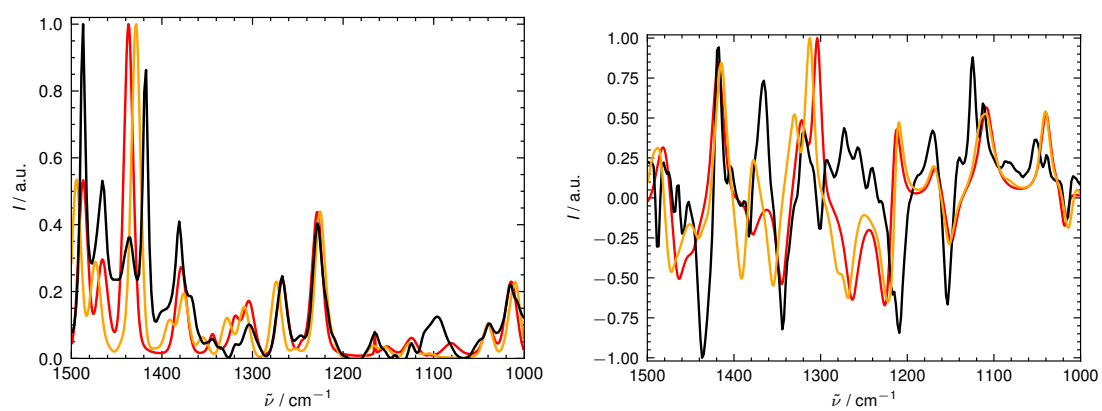


Figure S82: Aligned spectrum of compound **15**, isomer 0. Left: IR, Right: VCD.

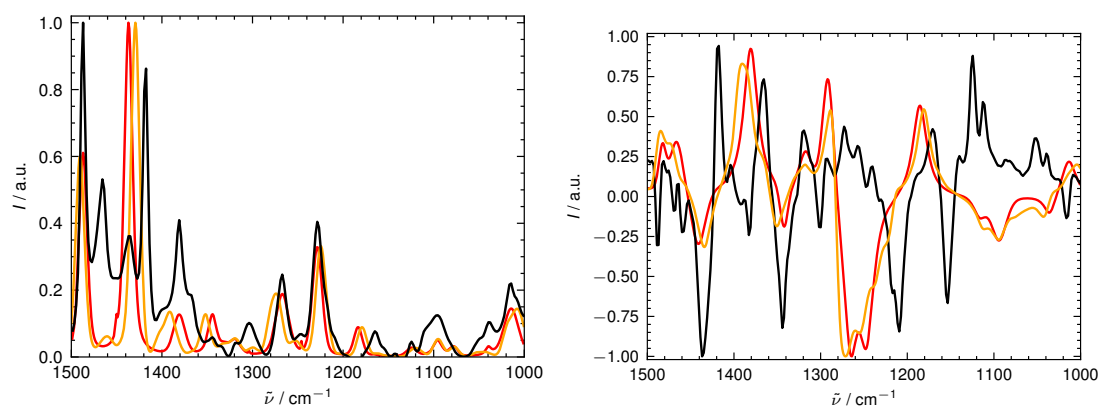


Figure S83: Aligned spectrum of compound **15**, isomer 1. Left: IR, Right: VCD.

3.16 Compound 16

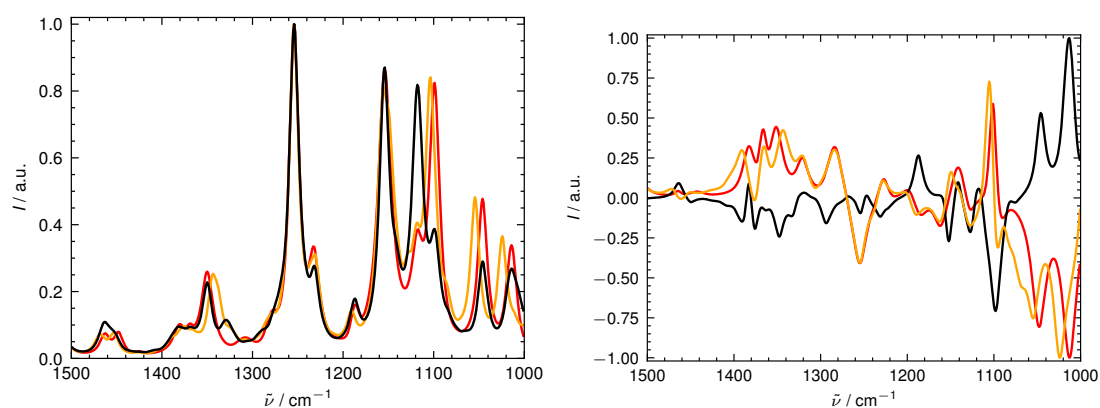


Figure S84: Aligned spectrum of compound **16**, isomer 0. Left: IR, Right: VCD.

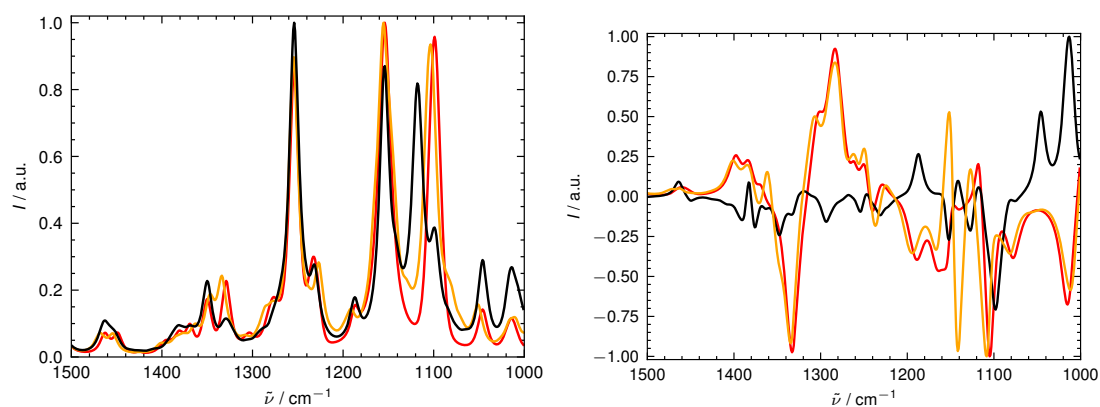


Figure S85: Aligned spectrum of compound **16** isomer 1. Left: IR, Right: VCD.

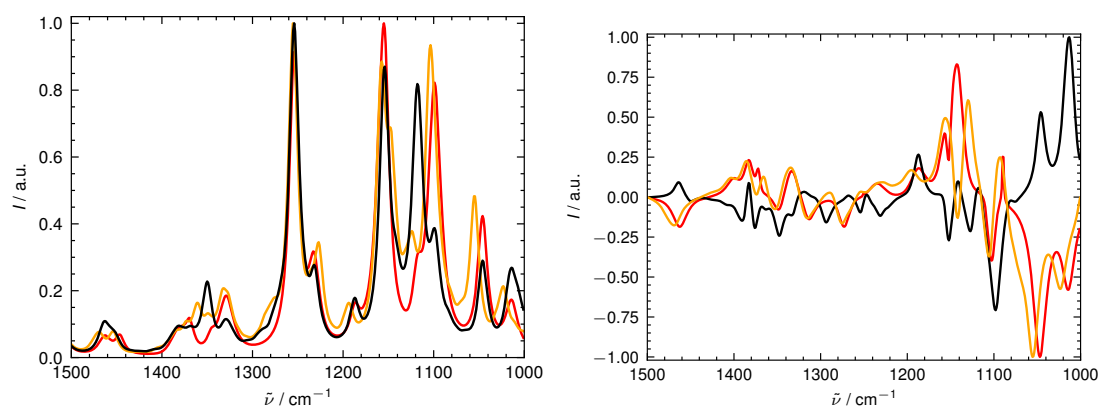


Figure S86: Aligned spectrum of compound **16** isomer 2. Left: IR, Right: VCD.

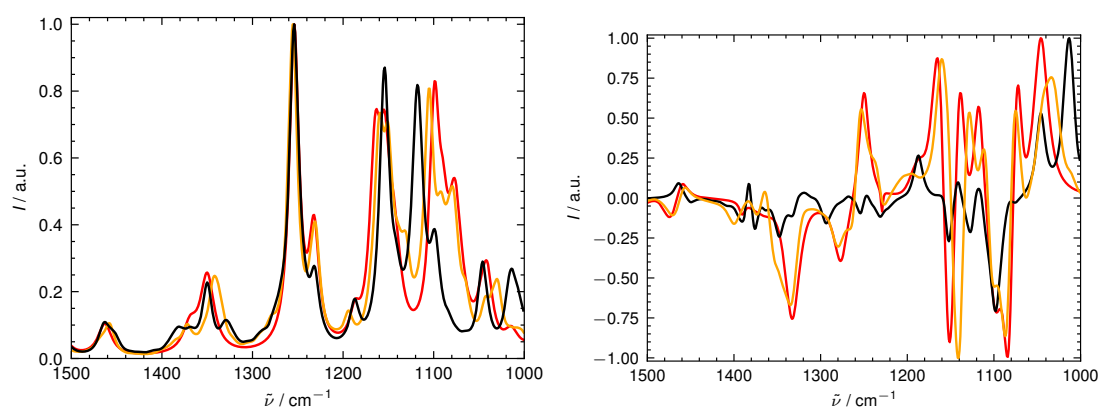


Figure S87: Aligned spectrum of compound **16** isomer 3. Left: IR, Right: VCD.

3.17 Compound 17

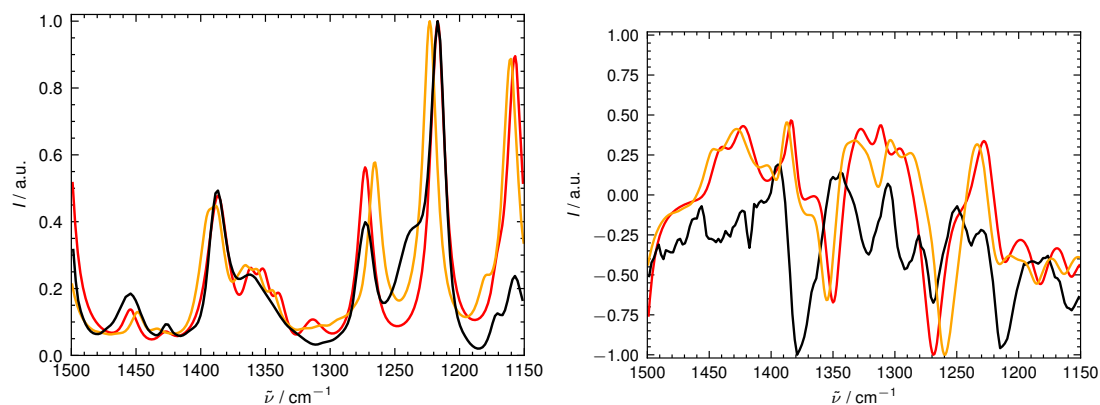


Figure S88: Aligned spectrum of compound **17**, isomer 0. Left: IR, Right: VCD.

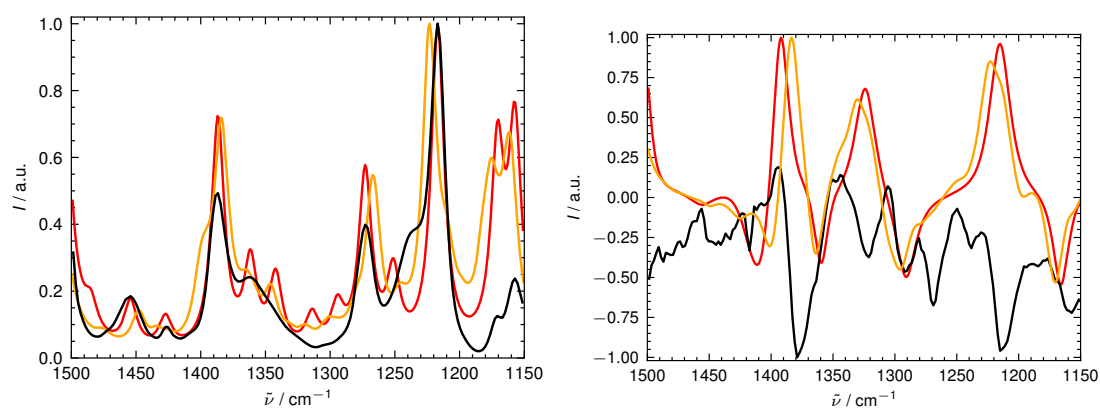


Figure S89: Aligned spectrum of compound **17** isomer 1. Left: IR, Right: VCD.

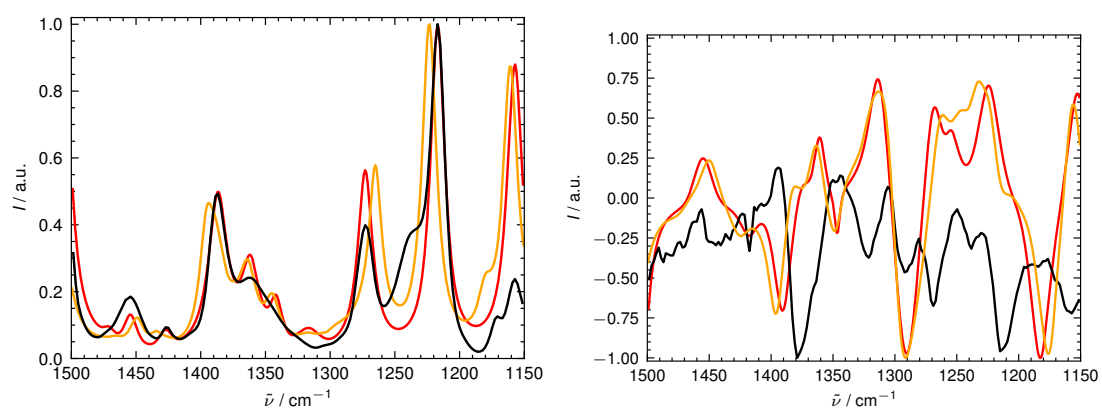


Figure S90: Aligned spectrum of compound **17** isomer 2. Left: IR, Right: VCD.

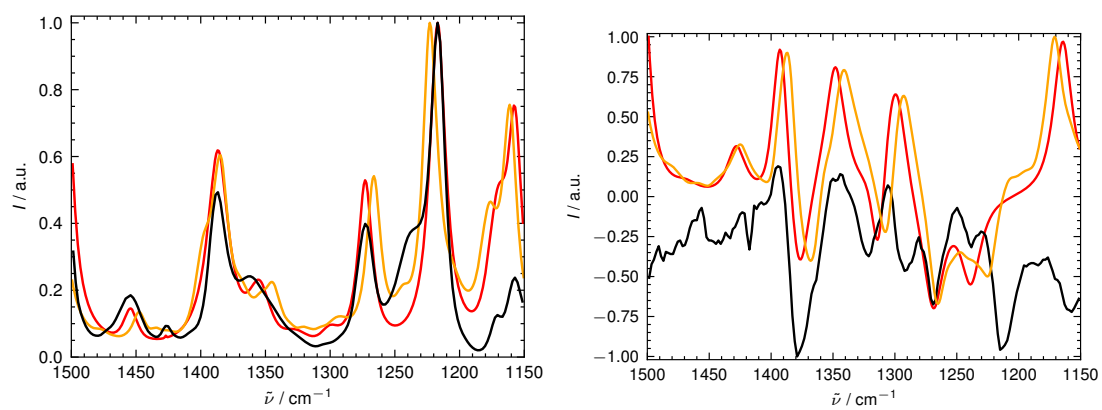


Figure S91: Aligned spectrum of compound **17** isomer 3. Left: IR, Right: VCD.