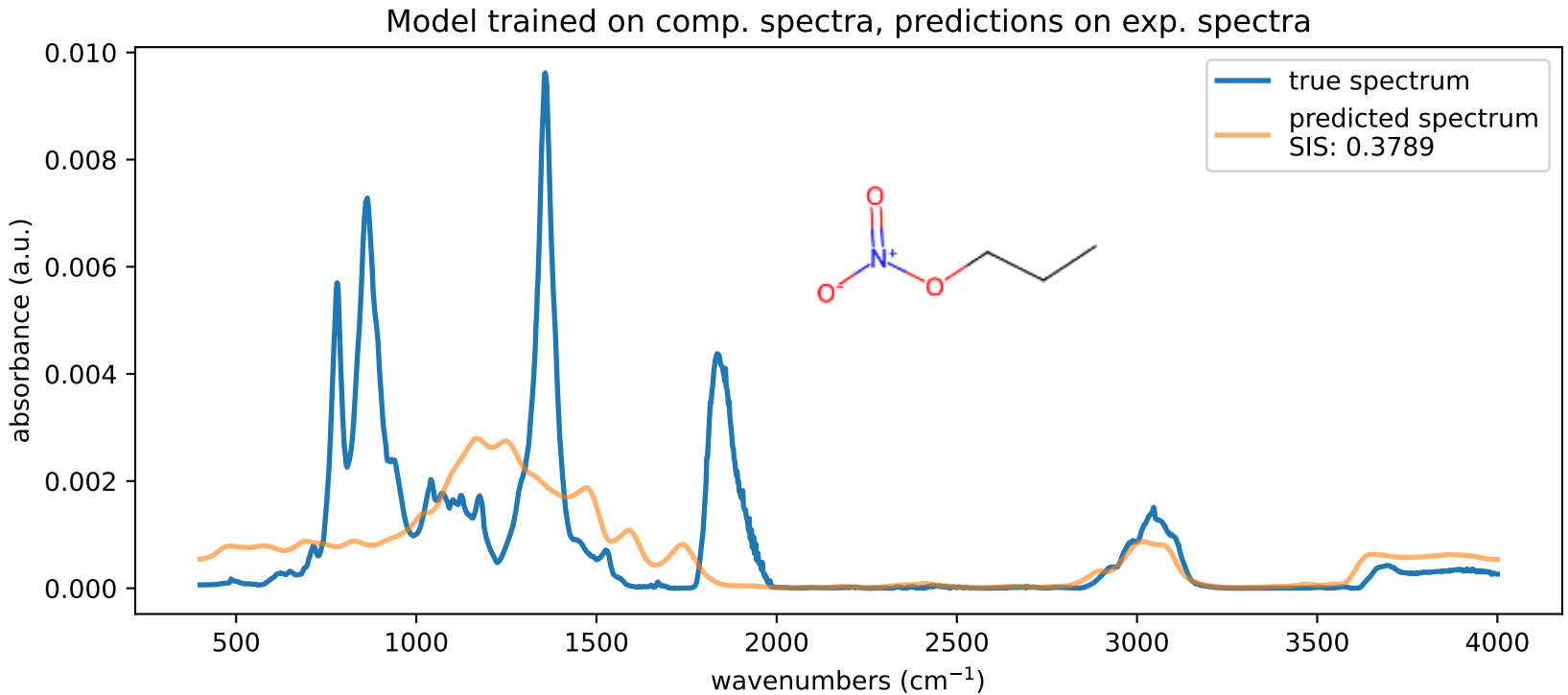
Model trained on comp. spectra, predictions on exp. spectra
true spectrum
predicted spectrum
SIS: 0.3789
absorbance (a.u.)
0.010
0.008
0.006
0.004
0.002
0.000
500
1000
1500
2000
2500
3000
3500
4000
wavenumbers (cm^{-1})
O
N+
O-
O