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Accessory Publication

Surface-Enhanced Raman Scattering Spectroscopy of Resveratrol

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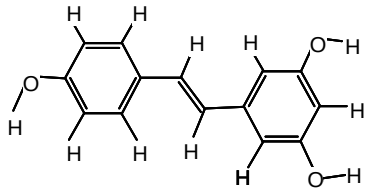
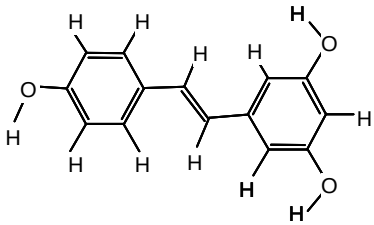
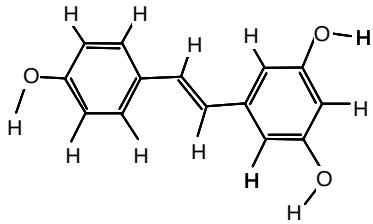
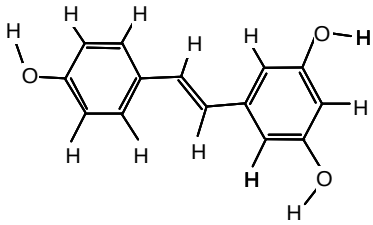
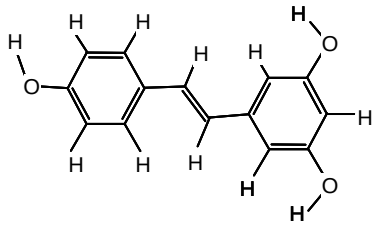
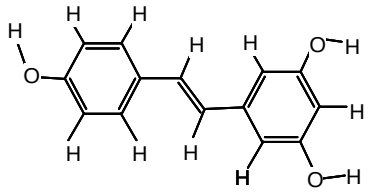
	Structure of conformers	relative energy (kJ mo^{l-1})	torsion angles
(a)		**+3.15**	C(5)-C(4)-C(8)-C(9) = -3.6º C(8)-C(9)-C(10)-C(15) = -4.1º
(b)		**+1.05**	C(5)-C(4)-C(8)-C(9) = -6.2º C(8)-C(9)-C(10)-C(15) = -8.7º
(c)		**+0.53**	C(5)-C(4)-C(8)-C(9) = -4.7º C(8)-C(9)-C(10)-C(15) = -6.3º
(d)		**0.00**	C(5)-C(4)-C(8)-C(9) = -4.2º C(8)-C(9)-C(10)-C(15) = -6.1º
(e)		**+0.79**	C(5)-C(4)-C(8)-C(9) = -5.4º C(8)-C(9)-C(10)-C(15) = -8.3º
(f)		**+2.89**	C(5)-C(4)-C(8)-C(9) = -2.9º C(8)-C(9)-C(10)-C(15) = -3.8º

Fig. S1: Relative energies and torsion angles of six different conformers of *trans*- resveratrol calculated using DFT calculations at B3LYP/6-31G(d) level.

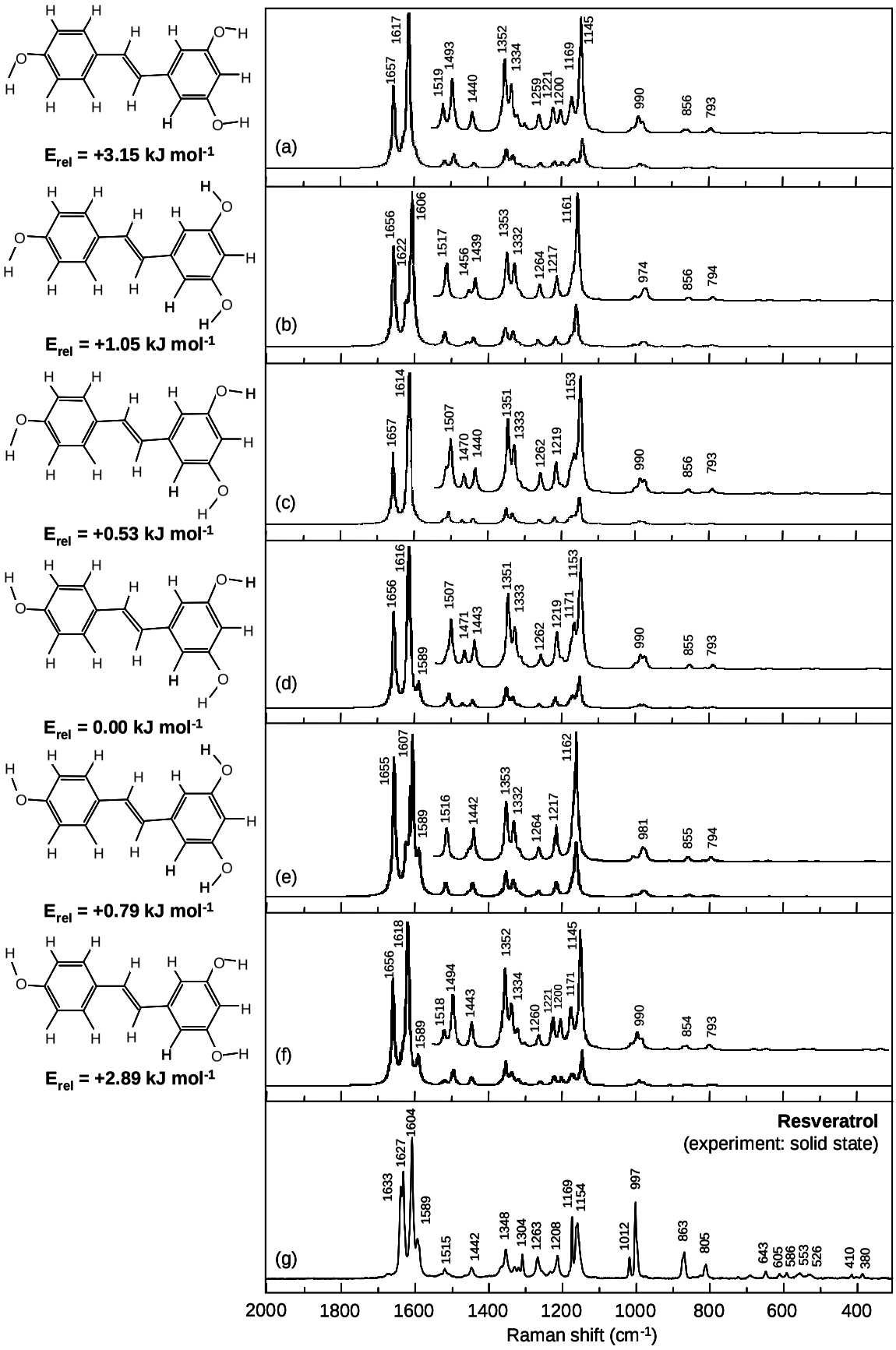

E_rel = +3.15 kJ mol-1
E_rel = +1.05 kJ mol-1
E_rel = +0.53 kJ mol-1
E_rel = 0.00 kJ mol-1
E_rel = +0.79 kJ mol-1
E_rel = +2.89 kJ mol-1
(a)
(b)
(c)
(d)
(e)
(f)
(g)
Resveratrol
(experiment: solid state)
2000 1800 1600 1400 1200 1000 800 600 400
Raman shift (cm-1)

Fig. S2: Predicted Raman spectra of the six different conformers of *trans*- resveratrol (a-f) obtained from DFT calculations at B3LYP/6-31G(d) level in comparison to the experimental solid-state Raman spectrum collected using a 782-nm excitation laser (g).

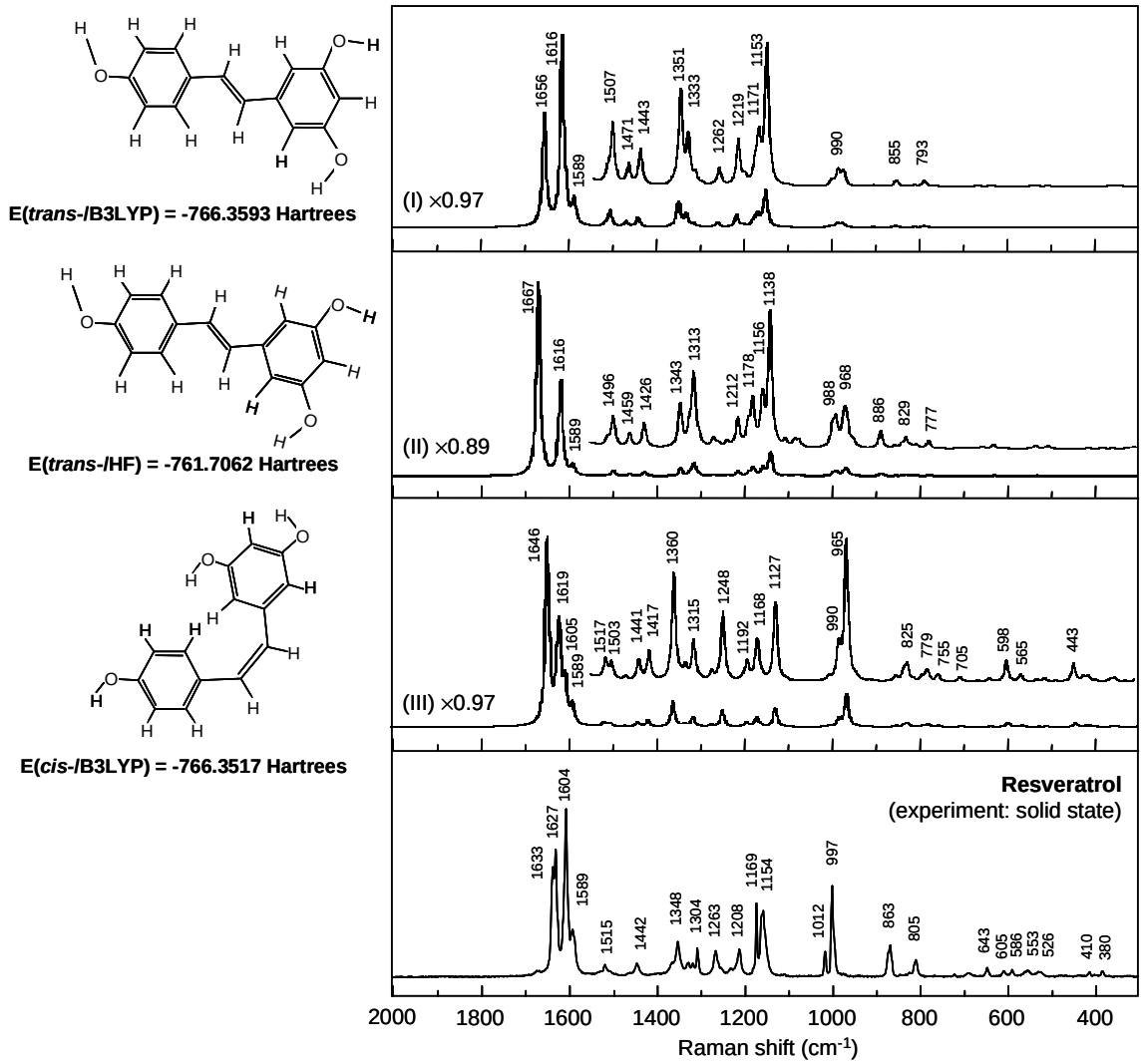


Fig. S3: Relative energies and predicted Raman spectra of *trans*-resveratrol obtained from two different methods—DFT (*I*) and Hartree-Focks (*II*) calculations—in comparison to those of *cis*- isomer calculated using DFT method at B3LYP/6-31G(d) level (*III*).

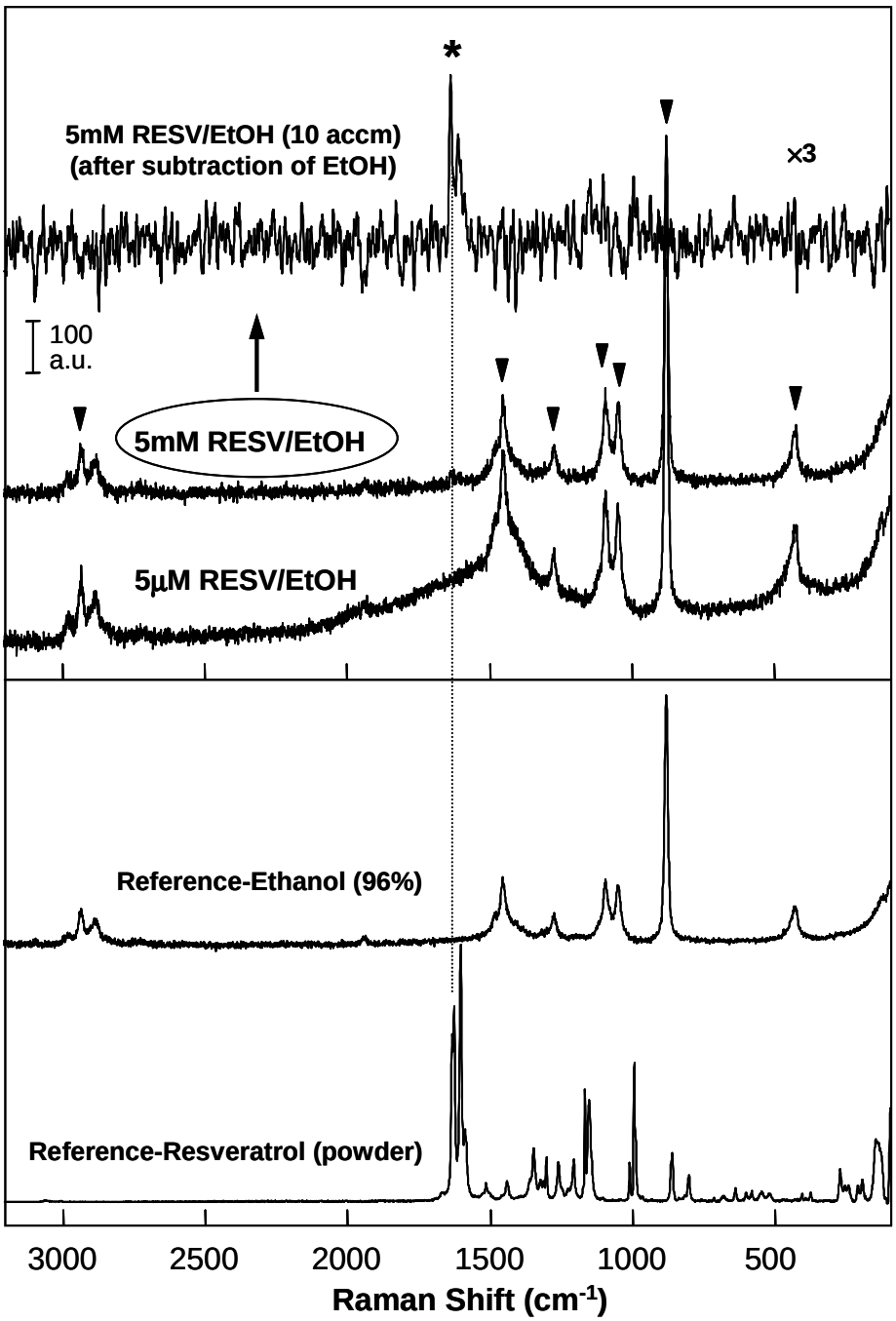


Fig. S4: Experimental Raman spectra of *trans*-resveratrol in 96% ethanol solution using 782-nm excitation laser in comparison to reference spectra of ethanol and *trans*-resveratrol. Bands marked by (▼) represents ethanol signatures, whereas the band marked by (*) reveals the existence of resveratrol disclosed after performing spectral subtraction to remove ethanol interference.