

Table S1. Frequency differences (S-R / cm^{-1}) of carboxy OH stretching between the phenolic OH rotamer

Computational level	B	X	I
B3LYP/cc-pVDZ	-0.36	+4.1	-0.95
CAM-B3LYP/6-31+G*	-0.87	+4.7	-0.40
CAM-B3LYP/cc-pVDZ	-0.28	+4.2	-0.66
CAM-B3LYP/cc-pVTZ	-0.44	+3.7	-0.18