

# Table S-V

Band <sup>#</sup>	cm <sup>-1</sup>	Vibrational origin	Ref. <sup>##</sup>
49*	1414	–COO <sup>-</sup> symmetric stretching in homocysteine	51
50	1438	CH <sub>2</sub> deformation & scissoring	45
51	1457	CH <sub>2</sub> wagging, CH <sub>2</sub> /CH <sub>3</sub> deformation	45
52	1488	CH <sub>2</sub> scissoring in tyrosine	50
53	1502	NH <sub>3</sub> symmetric bending in tyrosine	50
54	1515	C–C–H & C–N stretching in tyrosine	50
55	1528	C4=C5 stretching in imidazole ring of deprotonated histidine (imidazolate)	93
56	1546	C2=C3 stretching in pyrrole ring of tryptophan	93
57	1575	C4=C5 stretching in imidazole ring of $\tau$ histidine tautomer	93
57*	1584	C4=C5 stretching in imidazole ring of $\pi$ histidine tautomer	93
58	1598	–COO <sup>-</sup> asymmetric stretching in homocysteine NH <sub>3</sub> bending in methionine sulfoxide	51

<sup>#</sup>Numbers and colors are the same as those of the sub-bands shown in Fig. 8 of the main paper.

<sup>##</sup>Reference numbers are the same as those listed in the main paper.