Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary information

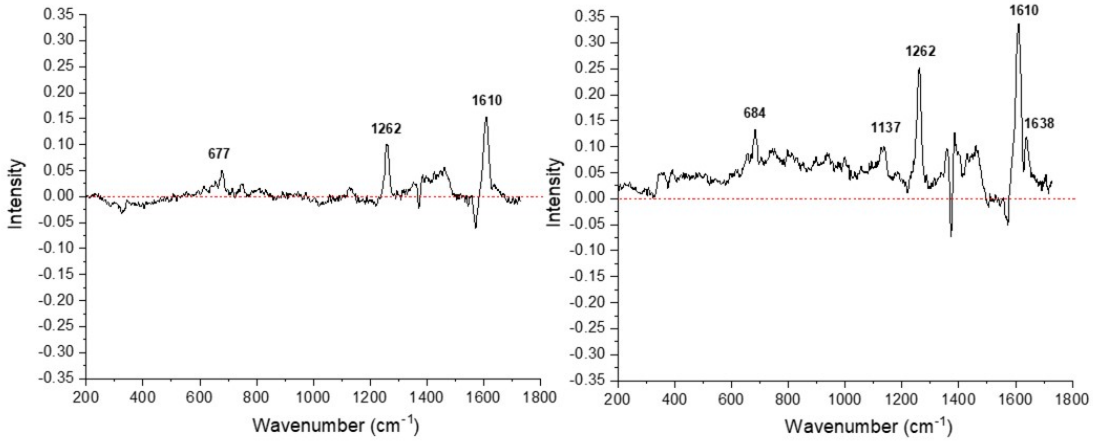

Fig. SI-1. Resonance Raman spectra subtraction of A) ZoPrX Ground State to H_2O_2-exposed state and B) ZoPrX Ground State to $H_2O_2(O^{18})$-exposed state.

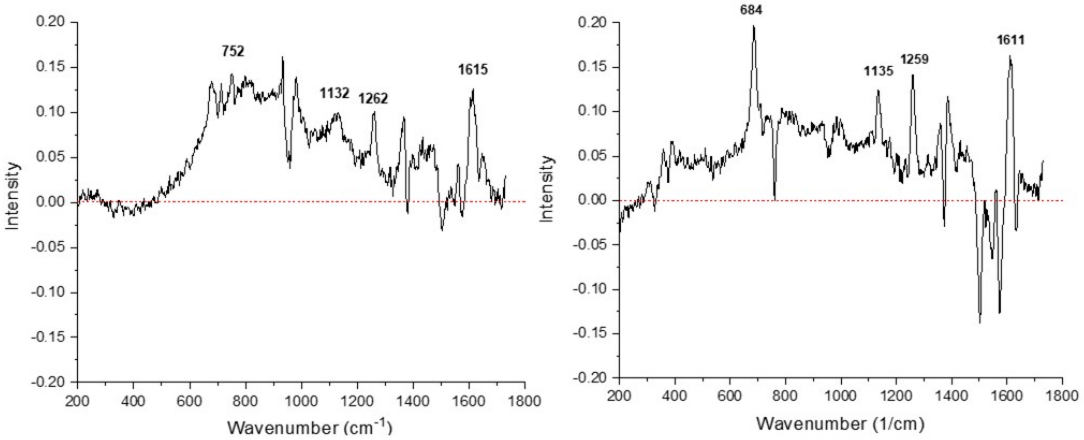

Fig. SI-2. Resonance Raman spectra subtraction of A) HRP Ground State to H_2O_2-exposed state and B) HRP Ground State to $H_2O_2(O^{18})$-exposed state.

ZoPX			HRP			Assignment	
Nativa	H_2O_2	H_2O_2 -O^{18}	Native	H_2O_2	H_2O_2 -O^{18}		
1631	1630	1630	1631	1630	1630	ν_{10} (B_{1g})	$\nu(C_\alpha C_m)_{asym}$
		1618			1618		ν(C=C)
	1613	1612				ν_{37} (E_u)	$\nu(C_\alpha C_m)_{asym}$
1572	1577	1577	1573	1573	1577	ν_{19} (A_{2g})	$\nu(C_\alpha C_m)_{asym}$
	1567	1568			1570	ν_2 (A_{2g})	$\nu(C_\beta C_\beta)$
		1560			1563	ν_{38} (E_u)	$\nu(C_\beta C_\beta)$
			1547	1547	1548	ν_{11} (B_{1g})	$\nu(C_\beta C_\beta)$
1505	1503	1505	1498	1500	1500	ν_3 (A_{1g})	$\nu(C_\alpha C_m)_{sym}$
1493	1490	1491				ν_3 (A_{1g})	$\nu(C_\alpha C_m)_{sym}$
1428	1427	1429	1429	1430	1431		$\delta s(=CH_2)$
1377	1377	1378	1375	1375	1376	ν_4 (A_{1g})	ν(Pyr half-ring)$_{sym}$
	1260	1260		1259	1259	$\nu_5 + \nu_9$ (A_{1g})	$\nu(C_\beta X)_{sym}$ & $\delta(C_\beta Y)_{sym}$
1238	1238	1238	1239	1239	1239	ν_{13} (B_{1g})	$\delta(C_m H)$
1177	1177	1177	1172	1172	1172	ν_{30} (B_{2g})	ν(Pyr half-ring)$_{asym}$
1132	1132	1132	1129	1129	1129	ν_{22} (A_{2g})	ν(Pyr half-ring)$_{asym}$
991	991	992	988	988	988	ν_{31} (B_{2g})	$\nu(C_\beta H)_{asym}$
932	932	932	932	932	932	ν_{46} (E_u)	δ(Pyr def)$_{asym}$
759	759	759	758	758	758	ν_{16} (B_{1g})	δ(Pyr def)$_{sym}$
719	719	719	720	720	720	ν_{24} (A_{2g})	δ(Pyr def)$_{asym}$
681	681	681	682	682	682	ν_7 (A_{1g})	δ(Pyr def)$_{sym}$
595	595	596	596	596	597	ν_{48} (E_u)	δ(Pyr def)$_{sym}$
	512	514				ν_{49} (E_u)	δ(Pyr rot)
442	439	438	441	438	444	ν_{33} (B_{2g})	δ(Pyr rot)
435	432	432		433		ν_{25} (A_{2g})	δ(Pyr rot)
		417			415	ν_{50} (E_u)	δ(Pyr rot)
410	410	410	410	410	409		$\delta(C_b C_\alpha C_\beta)$
383	383	385	383	383	385	$2\nu_{35}$ (A_{1g})	δ(Pyr transl)
350	350	353	352	349	355	ν_8 (A_{1g})	n(M-N)

Table SI-1 Resonance Raman band assignments.

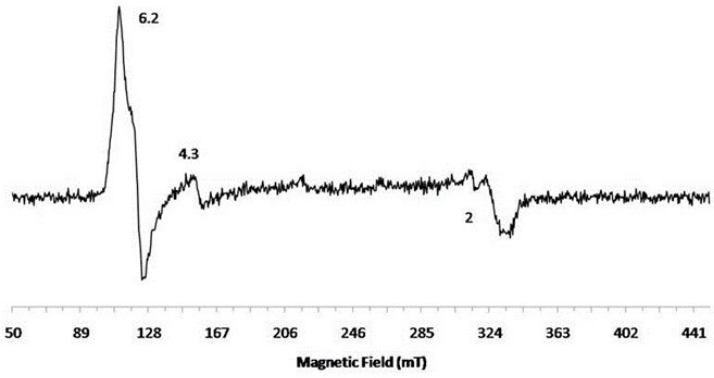

Figure SI-3. CW X-band EPR spectra of ZoPrx restored Ground State obtained at 17K after 72 h incubation at 4 °C in the presence of 1:10,000 Enzyme:H_2O_2 molar ratio.