

Supplementary Materials

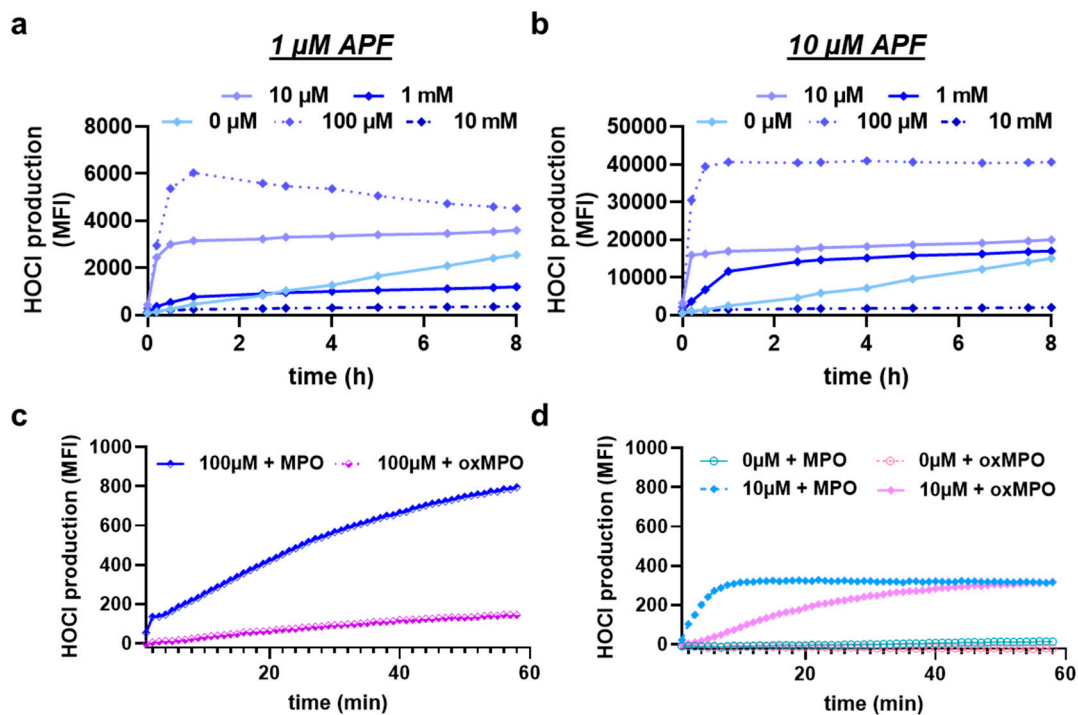


Figure S1. MPO activity is dependent on H₂O₂ and APF concentration. MPO was incubated with 0, 10, 100, 1000 or 10000 μ M H₂O₂ to measure HOCl production in the presence of (a) 1 μ M APF or (b) 10 μ M APF. (c, d) MPO and plasma-treated MPO were incubated with different concentrations of H₂O₂ to measure HOCl production.

modification	mass shift (m/z)	amino acids	fine control
+1O	15.9949	A. D. F. G. H. I. L. P. S. T. V. Y. C. E. K. M. N. Q. W. R	common
+2O	31.9898	F. H. I. L. P. S. T. V. Y. C. E. K. M. N. Q. W. R	common
+3O	47.9847	F. H. I. L. P. Y. C. E. K. M. N. Q. W. R	common
-2H+1O	13.9792	A. D. H. I. L. P. S. T. V. Y. C. E. K. M. N. Q. W. R	common
-1H-1N+1O	0.98401	Q. N	common
-1H+1N+2O	44.9850	A. D. F. G. H. I. L. P. S. T. V. Y. C. E. K. M. N. Q. W. R	common
-1H+1N+1O	28.9901	C. K. M. N. P. Q. W. Y. F	common
-1H+1N+3O	60.9799	F. I. L. Y. W	common
-1H+1N+4O	76.9749	F. Y. W	common
-2H+2O	29.9741	F. H. I. L. P. R. S. V. Y. C. K. M. Q. W	common
-2H+3O	45.9690	F. I. K. W. Y	common
-1C-1H-1N+2O	4.97893	H	common
-1H+1CI	33.9610	R. N. Q. H. K. F. W. Y	common
-2H	-2.01565	A. D. F. H. I. L. P. S. T. V. Y. C. E. K. M. N. Q. W. R	common
-4H	-4.03130	I. K. L. P. Q. S. T. V. W	common
-1C-2H-1O	-30.0105	D. E. P	common
-1C-5H-3N+1O	-43.0534	R	common
-1S	-31.9720	C	common
-2H-1S	-33.9877	C	common
-1S+1O	-15.9771	C	common
-2C-1H-1N+1O	-23.0159	H	common
-2C-2H-2N+2O	-22.0319	H	common
-1C-2H-2N+2O	-10.0319	H	common
-3H-1N+1O	-1.03163	K	common
+1C+2O	43.9898	K	common
+1C+1H+1N+1O	43.0058	K. C. D. E	common
-1C-4H-1S+1O	-32.0084	M	common
-1C-2H+3O	33.9690	M	common
-1C+1O	3.99491	W	common
-1C+2O	19.9898	W	common
-4H+2O	27.9585	W	common
-4H+3O	43.9534	W	common
+4O	63.9796	W	common
-2H+2CI	67.9220	W. Y. F	common
-2H+2N+4O	89.9701	W. Y. F	common

Figure S2. List of modifications used for PMI-Byonic.

Ar			Ar/O ₂			ArN ₂		
T mean	oxPTM	residue	T mean	oxPTM	residue	T mean	oxPTM	residue
0.85	+1O	M577	0.90	+1O	M688	0.42	+3O	C309
0.73	+1O	M453	0.67	+1O	M453	0.57	+3O	C398
0.67	+1O	M509	0.54	+1O	M519	0.37	+3O	C606
0.53	+1O	M588	0.53	+1O	M551	1.00	+3O	C663
0.45	+1O	M341	0.50	+1O	M409	0.14	+2O	C704
0.38	+1O	M472	0.44	+1O	M341	0.51	+3O	C704
0.36	+1O	M631	0.40	+1O	M644	0.15	+1O	F222
0.15	+1O	F222	0.35	+1O	M415	0.14	+1O	L539
0.14	+1O	L539	0.32	+1O	M253	0.13	+2O	L539
0.14	+2O	C704	0.31	+1O	M588	0.11	-2H+1O	M253
0.13	+2O	L539	0.19	+1O	L539	0.45	+1O	M341
1.00	+3O	C663	0.16	+1O	F222	0.73	+1O	M453
0.51	+3O	C704	0.13	+1O	P238	0.38	+1O	M472
0.42	+3O	C309	0.27	+2O	M577	0.67	+1O	M509
0.37	+3O	C606	0.25	+2O	M719	0.85	+1O	M577
0.10	-1C+1O	W535	0.18	+2O	C704	0.15	-1C-4H-1S+1O	M577
0.15	-1C-4H-1S+1O	M577	0.61	+3O	C398	0.53	+1O	M588
0.26	-1H-1N+1O	N331	0.36	+3O	C704	0.36	+1O	M631
0.11	-2H+1O	M253	0.15	-1C+1O	W535	0.26	-1H-1N+1O	N331
0.10	-2H+1O	Y723	0.19	-1C-4H-1S+1O	M588	0.10	-1C+1O	W535
			0.15	-1H-1N+1O	N331	0.10	-2H+1O	Y723
			0.14	-2H	L539			
			0.15	-2H+1O	W535			
			0.48	-2H-1S	C309			
			0.48	-2H-1S	C606			
			0.13	-2H+1O	M341			

Figure S3. Oxidative posttranslational modification found on MPO after plasma exposure. MPO was exposed to gas (control) or plasma, digested with trypsin and measured by Q-Exactive. The significance of the modification compared to gas control was determined using a custom R script that performed a Wilcoxon rank sum test with a cutoff of $p \leq 0.05$ (T mean).