Supplementary Information for:

Performance optimization and toxicity effects of the electrochemical oxidation of octogen

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Table S1. Kinetics and energy consumption of HMX degradation under different operating conditions.

Parameter	Factors	K (min^{-1})	R^2	Average voltage (V)	EC (kWh/g)
Electrolyte concentration (mol/L)	0.05	4.2×10^{-2}	0.985	6.19	2.22
	0.10	4.9×10^{-2}	0.931	5.27	1.81
	0.15	5.5×10^{-2}	0.935	4.15	1.33
	0.20	6.1×10^{-2}	0.947	3.95	1.16
	0.25	6.5×10^{-2}	0.956	3.68	1.03
Current density (mA/cm^2)	10.0	5.4×10^{-2}	0.996	3.34	0.50
	20.0	5.8×10^{-2}	0.989	3.65	1.05
	30.0	6.1×10^{-2}	0.992	3.92	1.67
	40.0	6.2×10^{-2}	0.996	4.49	2.49
	50.0	6.1×10^{-2}	0.993	4.90	3.34
	70.0	9.1×10^{-2}	0.995	5.58	4.47
Inter-electrode distance (cm)	0.5	8.4×10^{-2}	0.980	4.44	3.63
	1.0	8.7×10^{-2}	0.993	4.30	3.42
	1.5	7.0×10^{-2}	0.991	5.05	4.29
	2.0	7.5×10^{-2}	0.982	5.35	4.68
	2.5	7.4×10^{-2}	0.998	5.65	5.35
Initial pH	3.0	6.2×10^{-2}	0.992	4.65	4.13
	5.0	9.2×10^{-2}	0.991	5.25	4.07
	7.0	6.5×10^{-2}	0.965	5.07	4.77
	9.0	4.9×10^{-2}	0.991	5.42	5.48

Table S2. Main degradation intermediates of HMX.

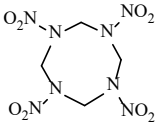
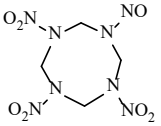
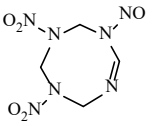
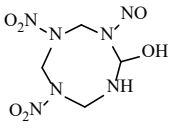
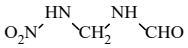
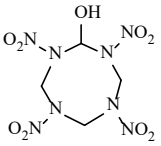
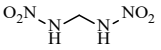
Mid product	M+[H]	Possible molecular formula	Molecular Structure	CAS
Original sample	297	$C_4H_8N_8O_8$		2691-41-0
I	281	$C_4H_8N_8O_7$		5755-28-2
II	234	$C_4H_7N_7O_5$		—
III	252	$C_4H_9N_7O_6$		—
IV	120	$C_2H_5N_3O_3$		479422-92-9
V	313	$C_4H_8N_8O_9$		—
VI	137	$CH_4N_4O_4$		14168-44-6

Table S3. Stress gene bank and its main functions.

Category		Gene selected	Known functions
Genotoxic Stress		*uvrA, recE, clpB, rnt, recX, ada, dinB, mutT, nfo, ding, ftsk, recN, sbmC, ybfE, dnaQ, mutH, mutM, mutS, mutY, yjiW, mug, yebG, sulA, lexA, polB, recA, ssb, umuD, uvrD, ruvA, uvrC, uvrY, polA*	DNA strand breaks and cross-linking, alter superhelicity, oxidative DNA damage, base alkylation, inhibition of DNA synthesis and replication
Redox Stress	Oxidation	*soxS, soxR, oxyR, inaA, dps, ahpF, katG, sodA, ahpC, katE, ytfE, katE, sodB, sodC, trxA*	Increased levels of superoxides, increased levels of peroxides, any other conditions, which alter the redox potential of the cell. Genes response to oxidative stress
	Detoxification	*norR, fpr, tam, yeiG, yafN, yeaE, grxA, gst*	
Protein Stress		*clpB, ycgE, cueR, entC, grpE, dnaK, fepB, dnaJ, rpoD, lon,ybgl*	Denaturation, misfolding, cross-linking and alkylation of proteins, oxidation of individual amino acids and protein damage.
Membrane Stress	Energy stress	*sdhC, cyoA*	Perturbations of electron transport and exposure to uncoupling agents, which affect ATP levels in the cell.
	Drug resistance	*yedW, dacA, dacB, marR, sbmA, bacA, yhjX, emrE, sanA, emrA, marC, mdtK, yajR, fsr, cmr, mrcB, pbpG, ssrA, ompC*	Related to compound /chemical induced stress, most product located or functioned at inner or outer membrane
	Metabolism	*flgM*、*motA*、*cyoA*	
	Cell Membrane	*amiC, clsA,*	Related to cell membrane and phospholipid synthesis
General Stress	Cold shock	*cspA, cspB*	Temperature downshift
	Cell killing	*dinJ,*、*slyA*、*yeeV*、 *yfjG*	
	General stress	*uspA, otsB, ydgL, bolA, rpoE,*	Disturbance of the biochemical and biophysical homeostasis of the cell.
	General	*phoB, crp, cdaR, ydeO, ybgI, gadX*	

Table S4. Single-factor experimental design.

No.	Electrolyte concentration (mol/L)	Current density （mA/cm^2）	Inter-electrode distance (cm)	Initial pH
1	0.05	20	2.0	7.0
2	0.10	20	2.0	7.0
3	0.15	20	2.0	7.0
4	0.20	20	2.0	7.0
5	0.25	20	2.0	7.0
6	0.25	10	2.0	7.0
7	0.25	20	2.0	7.0
8	0.25	30	2.0	7.0
9	0.25	40	2.0	7.0
10	0.25	50	2.0	7.0
11	0.25	70	2.0	7.0
12	0.25	70	0.5	7.0
13	0.25	70	1.0	7.0
14	0.25	70	1.5	7.0
15	0.25	70	2.0	7.0
16	0.25	70	3.0	7.0
17	0.25	70	1.0	3.0
18	0.25	70	1.0	5.0
19	0.25	70	1.0	7.0
20	0.25	70	1.0	9.0

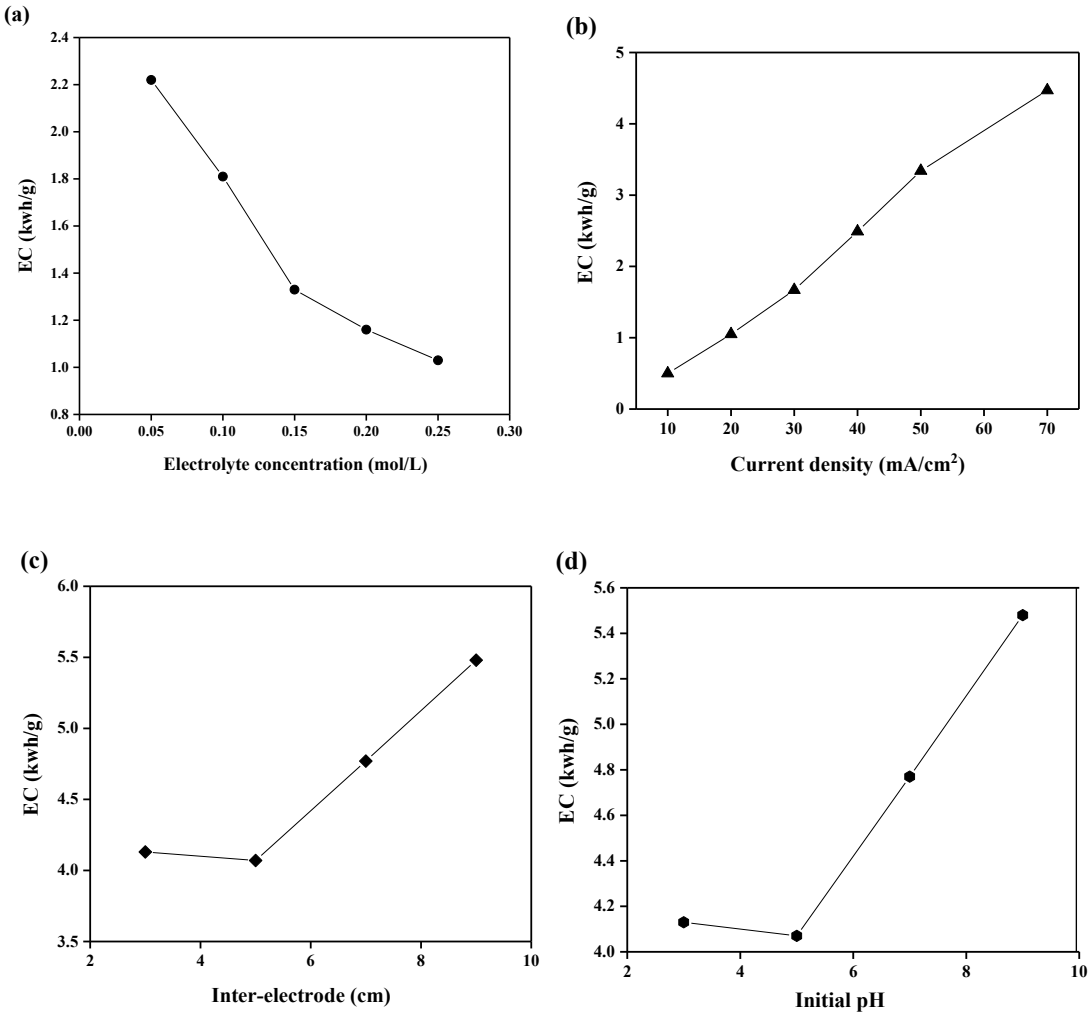
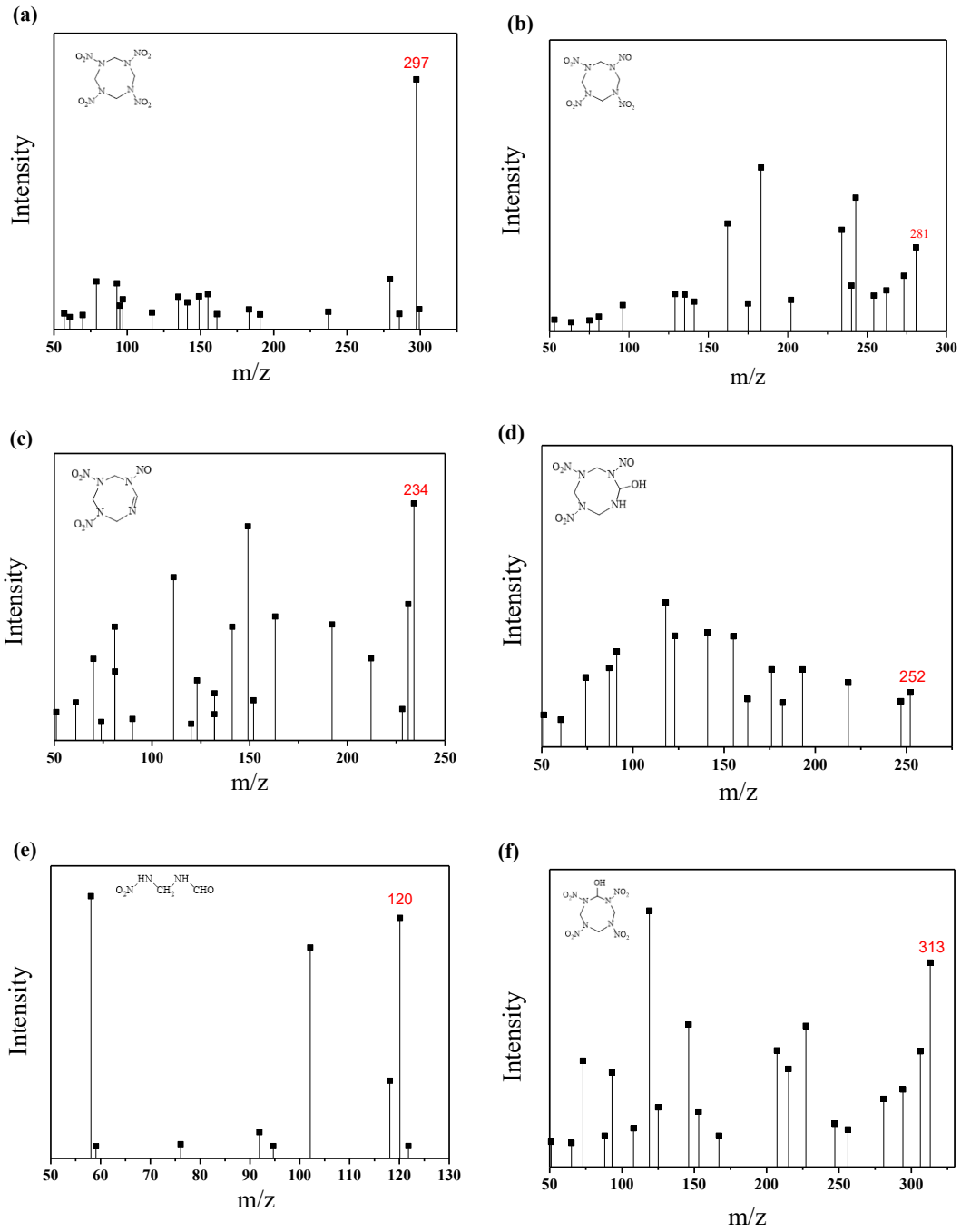


Figure S1. The energy consumption (EC) at different (a) electrolyte concentration, (b) current density, (c) inter-electrode, and (d) initial pH.


(a)
297
Intensity
m/z
(b)
281
Intensity
m/z
(c)
234
Intensity
m/z
(d)
252
Intensity
m/z
(e)
120
Intensity
m/z
(f)
313
Intensity
m/z

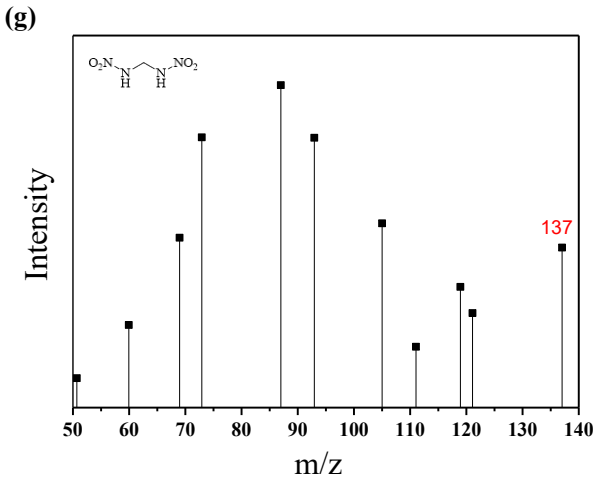


Figure S2. Ion spectra of HMX degradation intermediates in positive ion mode.

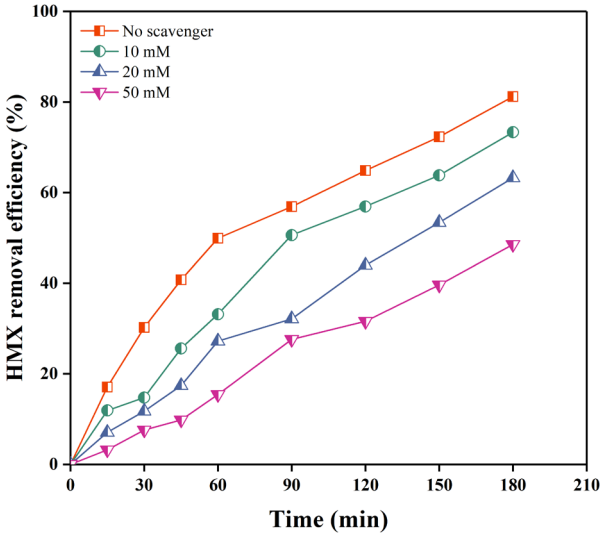


Figure S3. Removal of HMX under optimal conditions in the presence of different TBA concentrations.

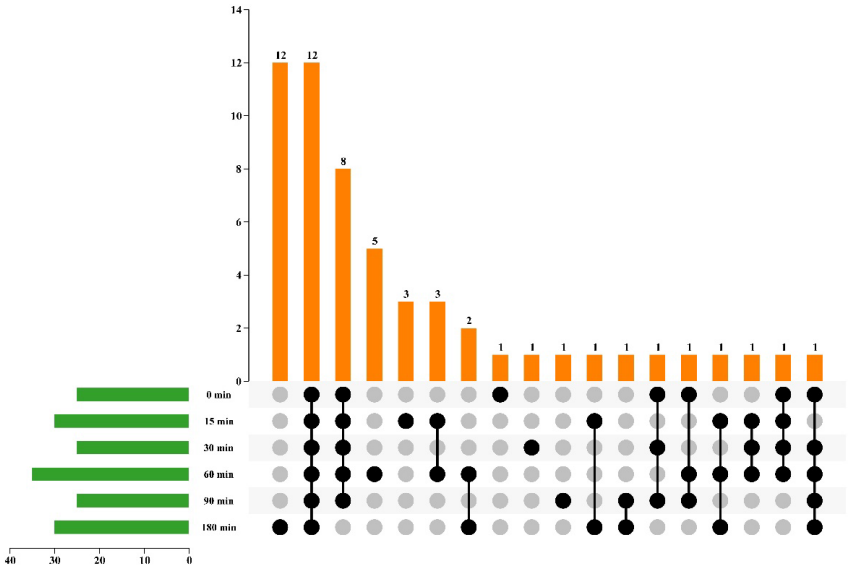


Figure S4. The number of genes showing altered expression ($TELI_{gene}$ > 1.5) during the electrochemical oxidation of HMX.

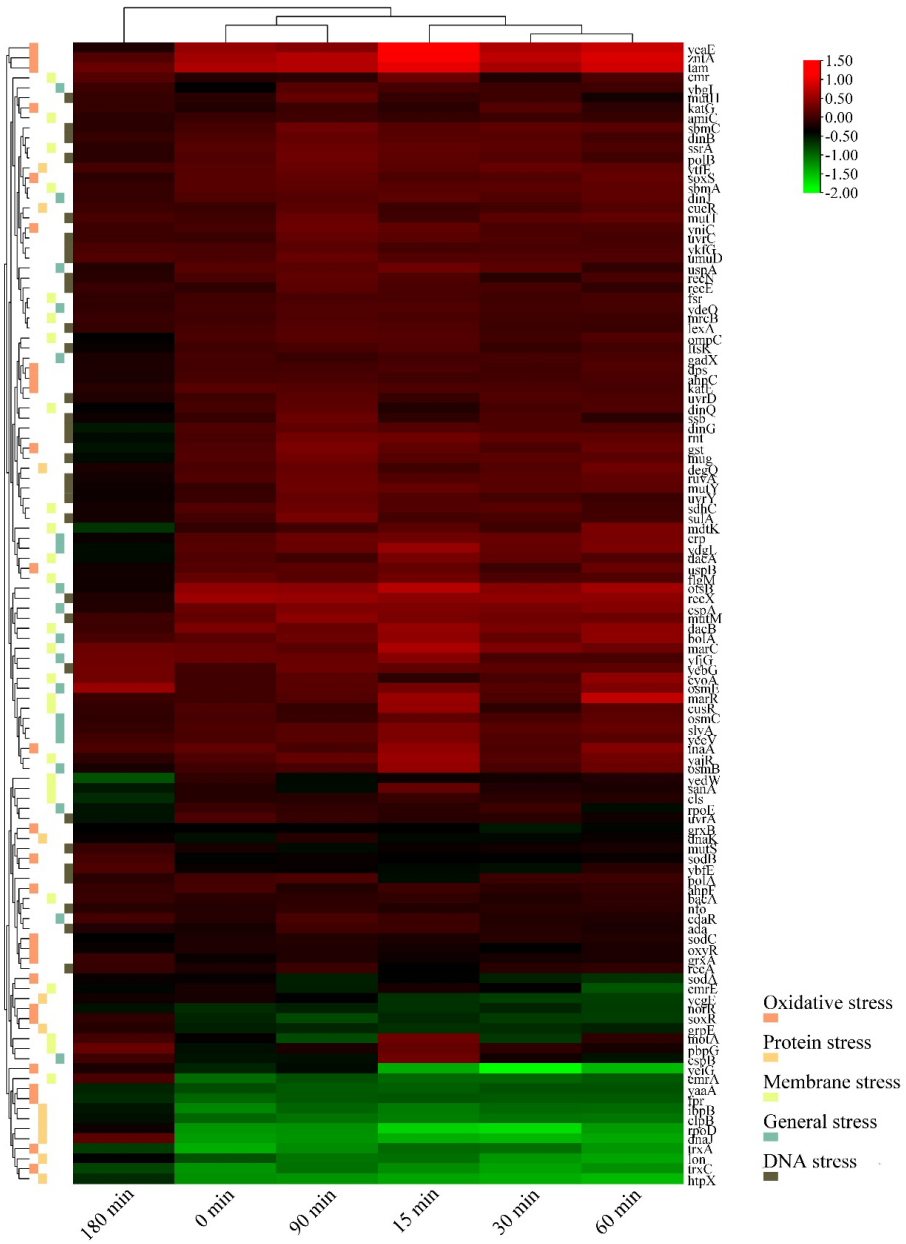


Figure S5. Hierarchical cluster (HCL) analysis diagram based on differential gene expressions (mean lnI, n = 3) of 114 selected stress genes in *E. coli* in exposure to the HMX samples at different times (Red colors indicate up-regulation, green colors indicate down-regulation).