water

Impact of Active Chlorines and •OH Radicals on Degradation of Quinoline Using the Bipolar Electro-Fenton Process

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Supplementary Materials

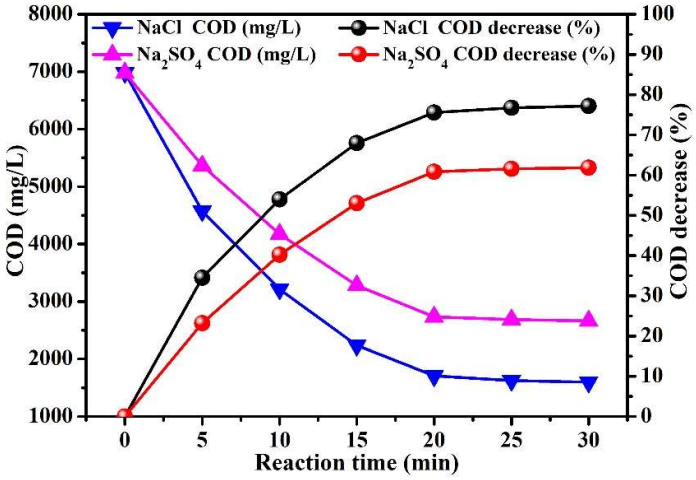


Figure S1. The effect of different supporting electrolytes on COD decrease efficiency of quinoline solution by E-Fenton process.

Table S1. Relationship between the COD of quinoline solution and reaction time.

Reaction Time	C_t (mg/L)	Ln (C_0/C_t)	$1/C_t-1/C_0$
0	6976	0.0000	0.0000000
2	5821	0.1810	0.0000284
5	4578	0.4212	0.0000751
10	3217	0.7740	0.0001675
15	2238	1.1369	0.0003035
20	1707	1.4077	0.0004425

Table S2. Kinetic parameters of COD degradation by E-Fenton process.

Reaction Orders	Linearized Form of Kinetic Model	Kinetic Equations	k	R^2
First-order kinetics	$\ln(C_0/C_t)=k_1t$	$\ln C_t=8.8092-0.0707t$	0.0707	0.9946
Second-order kinetics	$1/C_t-1/C_0=k_2t$	$1/C_t=(2.2074\times10^{-5})t+(1.2154\times10^{-4})$	2.2074×10^{-5}	0.9813

Table S3. Main intermediates during quinoline degradation identified by GC-MS.

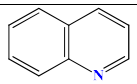
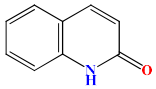
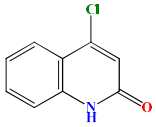
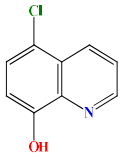
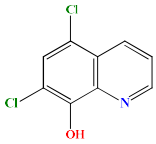
Symbol	Peak Time (min)	Compound	Molecular Formula	Chemical Structure	Reliability (%)
A	14.568	Quinoline	C_9H_7N		97.34
B	23.374	2(1H)-Quinolinone	C_9H_7NO		95.41
C	23.706	4-Chloro-2(1H)-quinolinone	C_9H_6ClNO		87.40
D	26.676	5-Chloro-8-hydroxyquinoline	C_9H_6ClNO		93.51
E	26.733	5,7-Dichloro-8-hydroxyquinoline	$C_9H_5Cl_2NO$		91.97

Table S4. Results of computational analysis for 8-hydroxyquinoline.

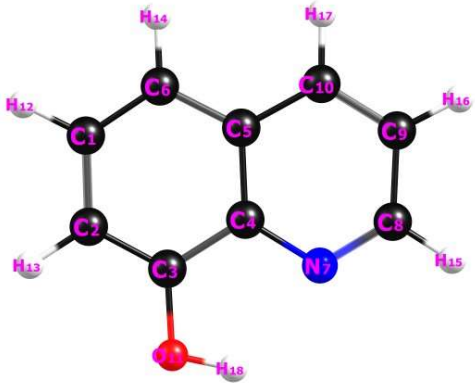
Structure and Numeration	Atoms	Fukui Function Indices		
		$f+$	$f-$	$f\,ave$
	C_1	0.07724	0.07944	0.07834
	C_2	0.06877	0.10718	0.08797
	C_3	0.06426	0.08640	0.07533
	C_4	0.07499	0.08144	0.07821
	C_5	0.07432	0.06699	0.07065
	C_6	0.06644	0.11336	0.08990
	N_7	0.10797	0.12242	0.11519
	C_8	0.11061	0.06475	0.08768
	C_9	0.09966	0.06703	0.08334
	C_{10}	0.12661	0.05167	0.08914
	O_{11}	0.01937	0.09652	0.05794
	H_{12}	0.01538	0.00745	0.01141
	H_{13}	0.01196	0.01013	0.01104
	H_{14}	0.01393	0.01193	0.01293
	H_{15}	0.01896	0.00985	0.01440
	H_{16}	0.01953	0.00738	0.01345
	H_{17}	0.02326	0.00623	0.01474
	H_{18}	0.00667	0.00975	0.00821

Table 5. Results of computational analysis for 5-chloro-8-hydroxyquinoline.

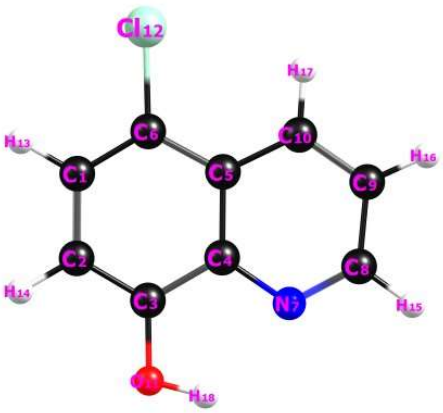
Structure and Numeration	Atoms	Fukui Function Indices		
		$f+$	$f-$	$f\,ave$
	C_1	0.07885	0.07415	0.07650
	C_2	0.06843	0.09393	0.08118
	C_3	0.06252	0.07948	0.07100
	C_4	0.07427	0.07080	0.07253
	C_5	0.07353	0.06128	0.06740
	C_6	0.07392	0.09608	0.08500
	N_7	0.10243	0.10750	0.10496
	C_8	0.10583	0.05664	0.08123
	C_9	0.09559	0.05983	0.07771
	C_{10}	0.11799	0.04605	0.08202
	O_{11}	0.01884	0.08858	0.05371
	Cl_{12}	0.04057	0.12060	0.08058
	H_{13}	0.01558	0.00622	0.01090
	H_{14}	0.01235	0.00870	0.01052
	H_{15}	0.01747	0.00862	0.01304
	H_{16}	0.01751	0.00659	0.01205
	H_{17}	0.01815	0.00612	0.01213
	H_{18}	0.00615	0.00883	0.00749

Table S6. Results of computational analysis for 5,7-dichloro-8-hydroxyquinoline.

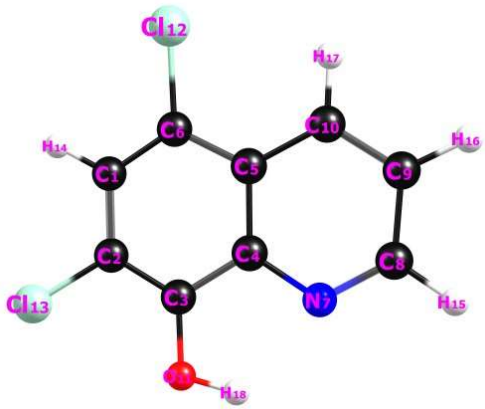
Structure and Numeration	Atoms	Fukui Function Indices		
		$f+$	$f-$	$f\,ave$
	C_1	0.08029	0.06922	0.07475
	C_2	0.07262	0.07888	0.07575
	C_3	0.06009	0.07467	0.09742
	C_4	0.07178	0.06171	0.06674
	C_5	0.07018	0.05544	0.06281
	C_6	0.07615	0.08001	0.07808
	N_7	0.09578	0.09747	0.09662
	C_8	0.10059	0.05015	0.07537
	C_9	0.08885	0.05539	0.07212
	C_{10}	0.11132	0.04092	0.07612
	O_{11}	0.01878	0.07641	0.04759
	Cl_{12}	0.04273	0.10478	0.07375
	Cl_{13}	0.04011	0.12259	0.08135
	H_{14}	0.01613	0.00558	0.01085
	H_{15}	0.01611	0.00766	0.01188
	H_{16}	0.01570	0.00604	0.01087
	H_{17}	0.01687	0.00537	0.01112
	H_{18}	0.00585	0.00766	0.00675

Table S7. Results of computational analysis for 2-picolinc acid.

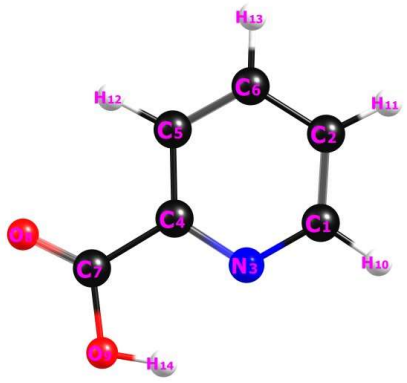
Structure and Numeration	Atoms	Fukui Function Indices		
		$f+$	$f-$	$f\,ave$
	C_1	0.11806	0.07293	0.09549
	C_2	0.12412	0.07303	0.09857
	N_3	0.13550	0.13978	0.13764
	C_4	0.12674	0.09095	0.10884
	C_5	0.12378	0.07757	0.10067
	C_6	0.13439	0.05114	0.09276
	C_7	0.07330	0.05908	0.06619
	O_8	0.05964	0.28868	0.17416
	O_9	0.02410	0.09791	0.06100
	H_{10}	0.01759	0.01139	0.01449
	H_{11}	0.01966	0.00807	0.01386
	H_{12}	0.01641	0.01116	0.01378
	H_{13}	0.02143	0.00698	0.01420
	H_{14}	0.00522	0.01132	0.00827

Table S8. Results of computational analysis for 2-hydroxyquinoline.

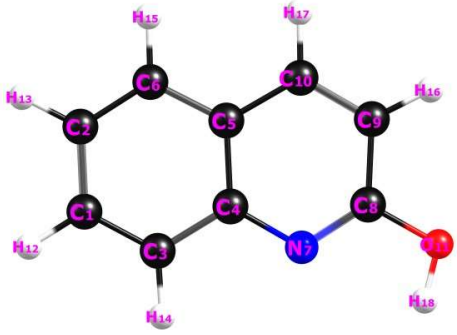
Structure and Numeration	Atoms	Fukui Function Indices		
		$f+$	$f-$	$f\,ave$
	C_1	0.08933	0.07854	0.08393
	C_2	0.07695	0.08732	0.08213
	C_3	0.08082	0.09736	0.08909
	C_4	0.07347	0.07673	0.07510
	C_5	0.06829	0.08083	0.07456
	C_6	0.09151	0.08699	0.08925
	N_7	0.07580	0.16466	0.12023
	C_8	0.07691	0.06405	0.07048
	C_9	0.10038	0.08199	0.09118
	C_{10}	0.12499	0.05303	0.08901
	O_{11}	0.02673	0.06918	0.04795
	H_{12}	0.01642	0.00810	0.01226
	H_{13}	0.01517	0.00861	0.01189
	H_{14}	0.01259	0.01064	0.01161
	H_{15}	0.01746	0.00971	0.01358
	H_{16}	0.01675	0.00956	0.01315
	H_{17}	0.02262	0.00600	0.01431
	H_{18}	0.01369	0.00665	0.01017

Table S9. Results of computational analysis for 2(1H)-quinolinone.

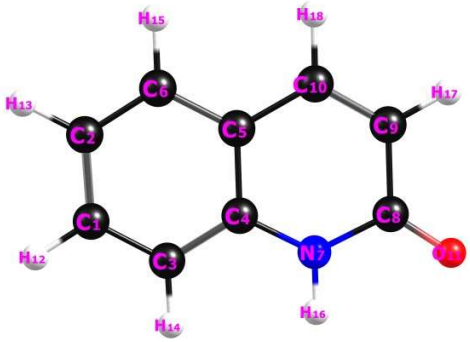
Structure and Numeration	Atoms	Fukui Function Indices		
		f+	*f*−	*f ave*
	C_1	0.09672	0.06116	0.07894
	C_2	0.07235	0.07535	0.07385
	C_3	0.08126	0.07657	0.07891
	C_4	0.07766	0.05782	0.06774
	C_5	0.07078	0.06424	0.06751
	C_6	0.09669	0.06643	0.08156
	N_7	0.04792	0.08649	0.06720
	C_8	0.06302	0.05446	0.05874
	C_9	0.10651	0.08654	0.09652
	C_{10}	0.11768	0.04742	0.08255
	O_{11}	0.04531	0.27465	0.15998
	H_{12}	0.01889	0.00585	0.01237
	H_{13}	0.01505	0.00726	0.01115
	H_{14}	0.01892	0.00695	0.01293
	H_{15}	0.01871	0.00619	0.01245
	H_{16}	0.01586	0.00820	0.01203
	H_{17}	0.01588	0.00830	0.01209
	H_{18}	0.02078	0.00616	0.01347

Table S10. Results of computational analysis for 4-chloro-2(1H)-quinolinone.

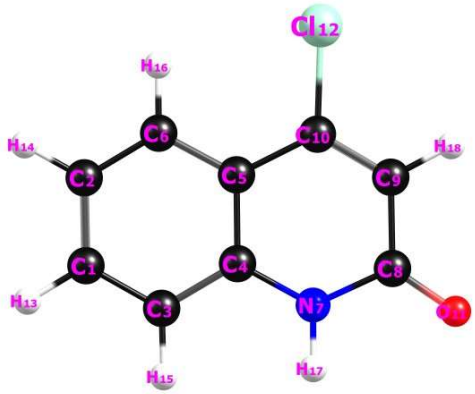
Structure and Numeration	Atoms	Fukui Function Indices		
		f+	*f*−	*f ave*
	C_1	0.09243	0.05539	0.07391
	C_2	0.06847	0.06991	0.06919
	C_3	0.07678	0.07051	0.07364
	C_4	0.07545	0.05202	0.06373
	C_5	0.06889	0.06022	0.06455
	C_6	0.09051	0.06134	0.07592
	N_7	0.04491	0.07941	0.06216
	C_8	0.05983	0.04994	0.05488
	C_9	0.10498	0.08517	0.09507
	C_{10}	0.12336	0.04342	0.08339
	O_{11}	0.04316	0.24974	0.14645
	Cl_{12}	0.05959	0.08343	0.07151
	H_{13}	0.01690	0.00531	0.01110
	H_{14}	0.01300	0.00679	0.00989
	H_{15}	0.01729	0.00639	0.01184
	H_{16}	0.01396	0.00633	0.01014
	H_{17}	0.01418	0.00735	0.01076
	H_{18}	0.01636	0.00740	0.01188

Table S11. Results of computational analysis for aniline.

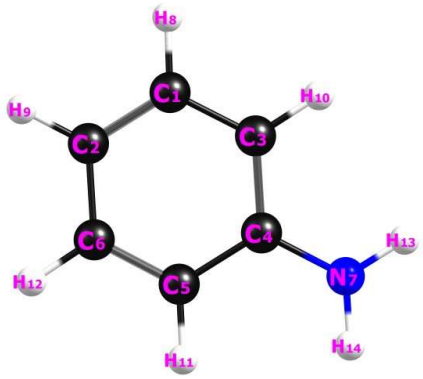
Structure and Numeration	Atoms	Fukui Function Indices		
		$f+$	$f-$	$f\,ave$
	C_1	0.12073	0.09253	0.10663
	C_2	0.09626	0.14909	0.12267
	C_3	0.11165	0.13891	0.12528
	C_4	0.09243	0.10415	0.09829
	C_5	0.11166	0.13891	0.12528
	C_6	0.12073	0.09253	0.10663
	N_7	0.06248	0.19748	0.12998
	H_8	0.03497	0.00791	0.02144
	H_9	0.02956	0.01398	0.02177
	H_{10}	0.04003	0.01195	0.02599
	H_{11}	0.04003	0.01195	0.02599
	H_{12}	0.03497	0.00791	0.02144
	H_{13}	0.05227	0.01633	0.03430
	H_{14}	0.05227	0.01633	0.03430

Table S12. Results of computational analysis for benzene.

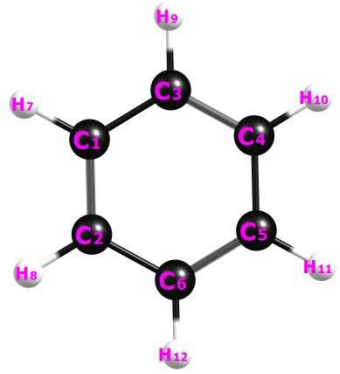
Structure and Numeration	Atoms	Fukui Function Indices		
		$f+$	$f-$	$f\,ave$
	C_1	0.13678	0.15143	0.14410
	C_2	0.13676	0.15142	0.14409
	C_3	0.13678	0.15144	0.14411
	C_4	0.13676	0.15142	0.14409
	C_5	0.13678	0.15143	0.14410
	C_6	0.13678	0.15144	0.14411
	H_7	0.02990	0.01524	0.02257
	H_8	0.02990	0.01524	0.02257
	H_9	0.02990	0.01525	0.02257
	H_{10}	0.02990	0.01524	0.02257
	H_{11}	0.02990	0.01524	0.02257
	H_{12}	0.02990	0.01525	0.02257

Table S13. The results of Mass balance and Cost calculation in E-Fenton process under the optimal process conditions.

Experimental Reagent	Reagent Dosage per Liter Solution	Types of Industrial Reagents	Industrial Reagents Consumption	Market Price of Industrial Reagents	Wastewater Treatment Cost per Ton
5 M H_2SO_4	3.0 ml/L	98 wt% H_2SO_4	1.501 kg/t	400 RMB/t	0.60 RMB/t
30 wt% H_2O_2	7.2 ml/L	30 wt% H_2O_2	7.992 kg/t	800 RMB/t	6.39 RMB/t
NaCl (AR)	3.0 g/L	NaCl (TP)	3.000 kg/t	500 RMB/t	1.50 RMB/t
5 M NaOH	5.0 mL/L	NaOH (TP)	2.415 kg/t	2500 RMB/t	2.50 RMB/t
2 wt‰ PAM	10.0 mL/L	PAM (TP)	20 g/t	9000 RMB/t	0.18 RMB/t
Electricity consumption		2.2 kW·h	Electricity cost		2.20 RMB/t
Estimated cost per ton of wastewater treatment				13.37 RMB/t=2.05 dollars/t	