# Supplementary material

# Activation of Sodium Percarbonate by Cysteine Complexation of Fe(II) for The Degradation of Acetaminophen in Water

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# Content

**Table S1** Fukui function values for each atom in the ACT molecule

| Atom | q(N-1) | q(N+1) | q(N) | $f_i^0$ | $f_i^-$ | $f_i^+$ |
|---|---|---|---|---|---|---|
| 1(C) | 0.0041 | -0.0989 | -0.0602 | 0.0515 | 0.0643 | 0.0387 |
| 2(C) | -0.0086 | -0.1428 | -0.0716 | 0.0671 | 0.0630 | **0.0712** |
| 3(C) | 0.1512 | -0.0122 | 0.0681 | **0.0817** | **0.0831** | **0.0802** |
| 4(C) | 0.0114 | -0.0966 | -0.0533 | 0.0540 | 0.0647 | 0.0433 |
| 5(C) | 0.0083 | -0.1286 | -0.0462 | **0.0685** | 0.0545 | **0.0824** |
| 6(C) | 0.1107 | -0.0203 | 0.0333 | 0.0655 | **0.0775** | 0.0536 |
| 7(H) | 0.0769 | 0.0091 | 0.0395 | 0.0339 | 0.0374 | 0.0304 |
| 8(H) | 0.0790 | -0.0008 | 0.0403 | 0.0399 | 0.0387 | 0.0411 |
| 9(H) | 0.0888 | 0.0166 | 0.0502 | 0.0361 | 0.0386 | 0.0336 |
| 10(H) | 0.0718 | 0.0111 | 0.0429 | 0.0303 | 0.0289 | 0.0317 |
| 11(N) | -0.0018 | -0.1057 | -0.0771 | 0.0520 | **0.0753** | 0.0286 |
| 12(H) | 0.1593 | 0.1006 | 0.1267 | 0.0294 | 0.0326 | 0.0262 |
| 13(C) | 0.2057 | 0.0657 | 0.1711 | **0.0700** | 0.0346 | **0.1055** |
| 14(C) | -0.0703 | -0.1220 | -0.0873 | 0.0258 | 0.0170 | 0.0347 |
| 15(H) | 0.0480 | 0.0062 | 0.0327 | 0.0209 | 0.0152 | 0.0266 |
| 16(H) | 0.0736 | 0.0085 | 0.0508 | 0.0326 | 0.0229 | 0.0423 |
| 17(H) | 0.0737 | 0.0087 | 0.0508 | 0.0325 | 0.0229 | 0.0421 |
| 18(O) | -0.2073 | -0.3965 | -0.2909 | **0.0946** | **0.0836** | **0.1056** |
| 19(O) | -0.0922 | -0.2522 | -0.1984 | **0.0800** | **0.1061** | 0.0538 |
| 20(H) | 0.2178 | 0.1503 | 0.1787 | 0.0337 | 0.0391 | 0.0284 |

**Table S2** Acetaminophen oxidation intermediates

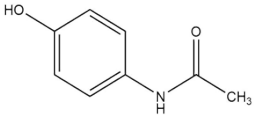
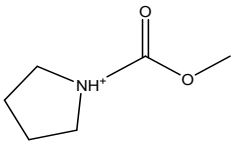
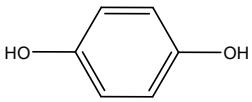
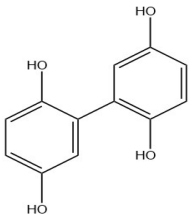
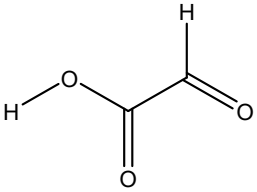
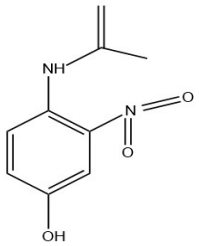
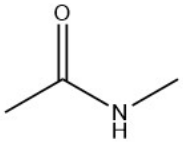
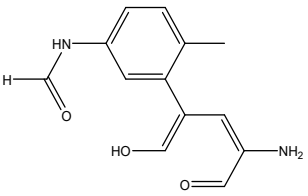
| Oxidation products | m/z | Chemical formula | Structure |
|---|---|---|---|
| Acetaminophen | 151 | $C_8H_9NO_2$ |  |
| P1 | 128 | $C_6H_{10}NO_2^+$ |  |
| P2 | 111 | $C_6H_6O_2$ |  |
| P3 | 218 | $C_{12}H_{10}O_4$ |  |
| P4 | 73 | $C_3H_7NO$ |  |
| P5 | 196 | $C_8H_8O_4N_2$ |  |
| P6 | 59 | $C_2H_5NO$ |  |
| P7 | 262 | $C_{13}H_{14}N_2O_4$ |  |

**Table S3** Prediction results of ACT and its oxidation product toxicity by T.E.S.T

| Substance | Fish 96h-LC50 | Water flea 48h-LC50 | Tetrahymena pyriformis 48h-IGC50 | Oral rat LD50（mg/kg） | bioaccumulation facto | Developmental Toxicity | Ames Mutagenicity |
|---|---|---|---|---|---|---|---|
| ACT | 71.26 | 26.05 | 187.68 | 1633.98 | 3.24 | 0.72 | 0.20 |
| P1 | 74.53 | 29.52 | 228.47 | 1892.95 | - | - | - |
| P2 | 35.32 | 12.92 | 98.51 | 369.99 | 11.80 | 0.63 | 0.08 |
| P3 | 15.6 | 10.89 | 33.87 | 2529.32 | 11.00 | 0.65 | 0.55 |
| P4 | 213.44 | 1022.18 | 218.75 | 1184.34 | - | 0.52 | 0.52 |
| P5 | 96.58 | 35.93 | 184.96 | 2734.58 | 1.51 | 0.64 | 0.80 |
| P6 | 802.98 | 347.72 | 4867.35 | 2865.25 | 0.60 | 0.77 | 0.03 |
| P7 | 62.21 | 20.58 | 133.76 | 616.44 | - | 0.86 | 0.57 |