**SUPPLEMENTARY INFORMATION**

**Singlet dioxygen 1O2, its generation, physico-chemical properties and its possible hormetic behavior in cancer therapy**

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**Computational details**

T = 298.15 K pH = 7.00 I = 0.25 M

πi0([H2aq]) = -0.55211 zJ·K-1 = 99.13 kJ·mol-1 \*1

∆πi'°{2H+ + 2e- = [H2aq]} = -0.55211 zJ·K-1 <=> pK = 17.37 <=> ∆G = 165 zJ = 99.13 kJ·mol-1

E'° = -514 mV

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([3O2aq]) = -0.09134 zJ·K-1 = 16.40 kJ·mol-1 \*1

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*2

∆πi'°{[3O2aq] + 4H+ + 4e- = 2\*[H2O]} = 1.82521 zJ·K-1 <=> pK = -57.41 <=> ∆G = -544 zJ = -327.72 kJ·mol-1

E'° = 849 mV

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([H2aq]) = -0.55211 zJ·K-1 = 99.13 kJ·mol-1 \*2

πi0 ([3O2aq]) = -0.09134 zJ·K-1 = 16.40 kJ·mol-1 \*1

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*2

∆πi'°{2\*[H2aq] + [3O2aq] = 2\*[H2O]} = 2.92943 zJ·K-1 <=> pK = -92.15 <=> ∆G = -873 zJ = -525.98 kJ·mol-1

T = 298.15 K pH = 0.00 I = 0.00 M

πi0 ([Haq]•) = -1.24199 zJ·K-1 = 223.00 kJ·mol-1 \*1

∆πi'°{H+ + e- = [Haq]•} = -1.24199 zJ·K-1 <=> pK = 39.07 <=> ∆G = 370 zJ = 223.00 kJ·mol-1

E'° = -2.31 V

T = 298.15 K pH = 0.00 I = 0.00 M

πi0 ([HO]•) = -0.14648 zJ·K-1 = 26.30 kJ·mol-1 \*1

πi0 ([H2O]) = 1.32102 zJ·K-1 = -237.19 kJ·mol-1 \*1

∆πi'°{[HO]• + H+ + e- = [H2O]} = 1.46750 zJ·K-1 <=> pK = -46.16 <=> ∆G = -438 zJ = -263.49 kJ·mol-1

E'° = 2.73 V

T = 298.15 K pH = 0.00 I = 0.00 M

πi0 ([3O2g]) = -0.00000 zJ·K-1 = 0.00 kJ·mol-1 \*1

πi0 ([H2g]) = -0.00000 zJ·K-1 = 0.00 kJ·mol-1 \*2

πi0 ([H2O]) = 1.32102 zJ·K-1 = -237.19 kJ·mol-1 \*2

∆πi'°{[3O2g] + 2\*[H2g] = 2\*[H2O]} = 2.64205 zJ·K-1 <=> pK = -83.11 <=> ∆G = -788 zJ = -474.38 kJ·mol-1

T = 298.15 K pH = 0.00 I = 0.00 M

πi0 ([1O2g]) = -0.52665 zJ·K-1 = 94.56 kJ·mol-1 \*1

πi0 ([H2g]) = -0.00000 zJ·K-1 = 0.00 kJ·mol-1 \*2

πi0 ([H2O]) = 1.32102 zJ·K-1 = -237.19 kJ·mol-1 \*2

∆πi'°{[1O2g] + 2\*[H2g] = 2\*[H2O]} = 3.16870 zJ·K-1 <=> pK = -99.67 <=> ∆G = -945 zJ = -568.94 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.00 M

πi0 (NAD+) = 6.55495 zJ·K-1 = -1176.94 kJ·mol-1 \*1

πi0 (NADH) = 6.20961 zJ·K-1 = -1114.94 kJ·mol-1 \*1

∆πi'°{NAD+ + H+ + 2e- = NADH} = -0.34534 zJ·K-1 <=> pK = 10.86 <=> ∆G = 103 zJ = 62.01 kJ·mol-1

E'° = -321 mV

T = 298.15 K pH = 7.00 I = 0.00 M

πi0 (NADP+) = 11.50677 zJ·K-1 = -2066.04 kJ·mol-1 \*1

πi0 (NADPH) = 11.16143 zJ·K-1 = -2004.04 kJ·mol-1 \*1

∆πi'°{NADP+ + H+ + 2e- = NADPH} = -0.34534 zJ·K-1 <=> pK = 10.86 <=> ∆G = 103 zJ = 62.01 kJ·mol-1

E'° = -321 mV

T = 298.15 K pH = 7.00 I = 0.25 M

πi0(adp) = 7.93486 zJ·K-1 = -1424.71 kJ·mol-1 \*1

πi0 (Pi) = 5.90080 zJ·K-1 = -1059.49 kJ·mol-1 \*1

πi0 (atp) = 12.76803 zJ·K-1 = -2292.50 kJ·mol-1 \*1

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*1

∆πi'°{adp + Pi = atp + [H2O]} = -0.20070 zJ·K-1 <=> pK = 6.31 <=> ∆G = 60 zJ = 36.04 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([O3]) = -0.96965 zJ·K-1 = 174.10 kJ·mol-1 \*1

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*1

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1 \*1

∆πi'°{[O3] + [H2O] = [1O2] + [H2O2]} = -0.22868 zJ·K-1 <=> pK = 7.19 <=> ∆G = 68 zJ = 41.06 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([O3]) = -0.96965 zJ·K-1 = 174.10 kJ·mol-1 \*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1 \*1

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*2

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*1

∆πi'°{[O3] + [H2O2] = 2\*[1O2] + [H2O]} = 0.29663 zJ·K-1 <=> pK = -9.33 <=> ∆G = -88 zJ = -53.26 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([HO2]•) = -0.18370 zJ·K-1 = 32.98 kJ·mol-1 \*1

πi0 ([HO]•) = -0.37352 zJ·K-1 = 67.07 kJ·mol-1 \*1

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*1

∆πi'°{[HO2]• + [HO]• = [1O2] + [H2O]} = 0.80038 zJ·K-1 <=> pK = -25.18 <=> ∆G = -239 zJ = -143.71 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([HO2]•) = -0.18370 zJ·K-1 = 32.98 kJ·mol-1 \*2

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1 \*1

∆πi'°{2\*[HO2]• = [1O2] + [H2O2]} = 0.03602 zJ·K-1 <=> pK = -1.13 <=> ∆G = -11 zJ = -6.47 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([HO2]•) = -0.18370 zJ·K-1 = 32.98 kJ·mol-1 \*1

πi0 ([HO]•) = -0.37352 zJ·K-1 = 67.07 kJ·mol-1 \*1

πi0 ([3O2aq]) = -0.09134 zJ·K-1 = 16.40 kJ·mol-1 \*1

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*1

∆πi'°{[HO2]• + [HO]• = [3O2aq] + [H2O]} = 1.33282 zJ·K-1 <=> pK = -41.92 <=> ∆G = -397 zJ = -239.31 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([HO2]•) = -0.18370 zJ·K-1 = 32.98 kJ·mol-1 \*2

πi0 ([3O2aq]) = -0.09134 zJ·K-1 = 16.40 kJ·mol-1 \*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1 \*1

∆πi'°{2\*[HO2]• = [3O2aq] + [H2O2]} = 0.56846 zJ·K-1 <=> pK = -17.88 <=> ∆G = -169 zJ = -102.07 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([HOCl]) = 0.22429 zJ·K-1 = -40.27 kJ·mol-1 \*2

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 ([Cl]-) = 0.73538 zJ·K-1 = -132.04 kJ·mol-1 \*2

∆πi'°{2\*[HOCl] = [1O2] + 2\*[Cl]-} = 0.39840 zJ·K-1 <=> pK = -12.53 <=> ∆G = -119 zJ = -71.53 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1 \*1

πi0 ([HOCl]) = 0.22429 zJ·K-1 = -40.27 kJ·mol-1 \*1

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 ([Cl]-) = 0.73538 zJ·K-1 = -132.04 kJ·mol-1 \*1

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*1

∆πi'°{[H2O2] + [HOCl] = [1O2] + [Cl]- + [H2O]} = 0.46186 zJ·K-1 <=> pK = -14.53 <=> ∆G = -138 zJ = -82.93 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 (UQ10H2) = -25.22108 zJ·K-1 = 4528.45 kJ·mol-1 \*1

πi0 (UQ10) = -25.28740 zJ·K-1 = 4540.36 kJ·mol-1 \*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1 \*1

∆πi'°{[1O2] + UQ10H2 = UQ10 + [H2O2]} = 0.84985 zJ·K-1 <=> pK = -26.73 <=> ∆G = -253 zJ = -152.59 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 (vitC) = 3.03142 zJ·K-1 = -544.29 kJ·mol-1 \*1

πi0 (DHA4) = 3.83413 zJ·K-1 = -688.42 kJ·mol-1 \*1

πi0 ([HO]•) = -0.37352 zJ·K-1 = 67.07 kJ·mol-1 \*2

∆πi'°{[1O2] + vitC = DHA4 + 2\*[HO]•} = 0.67946 zJ·K-1 <=> pK = -21.37 <=> ∆G = -203 zJ = -122.00 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 (vitC) = 3.03142 zJ·K-1 = -544.29 kJ·mol-1 \*1

πi0 (DHA4) = 3.83413 zJ·K-1 = -688.42 kJ·mol-1 \*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1 \*1

∆πi'°{[1O2] + vitC = DHA4 + ([H2O2]} = 1.71889 zJ·K-1 <=> pK = -54.07 <=> ∆G = -512 zJ = --308.63 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 (cytcred) = 0.15455 zJ·K-1 = -27.75 kJ·mol-1 \*1

πi0 ([HO2]•) = -0.18370 zJ·K-1 = 32.98 kJ·mol-1 \*1

πi0 (cytcox) = 0.04059 zJ·K-1 = -7.29 kJ·mol-1 \*1

∆πi'°{[1O2] + cytcred = [HO2]• + cytcox} = 0.32612 zJ·K-1 <=> pK = -10.26 <=> ∆G = -97 zJ = -58.55 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 (RH2lipoate) = -1.77480 zJ·K-1 = 318.67 kJ·mol-1 \*1

πi0 (Rlipoate) = -1.45613 zJ·K-1 = 261.45 kJ·mol-1 \*1

πi0 ([HO]•) = -0.37352 zJ·K-1 = 67.07 kJ·mol-1 \*2

∆πi'°{[1O2] + RH2lipoate = Rlipoate + 2\*[HO]•} = 0.19541 zJ·K-1 <=> pK = -6.15 <=> ∆G = -58 zJ = -35.09 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 ([GSH]) = 1.52051 zJ·K-1 = -273.01 kJ·mol-1 \*2

πi0 ([HO]•) = -0.37352 zJ·K-1 = 67.07 kJ·mol-1 \*2

πi0 ([GSSG]) = 3.33710 zJ·K-1 = -599.18 kJ·mol-1 \*1

∆πi'°{[1O2] + 2\*[GSH] = 2\*[HO]• + [GSSG]} = 0.17282 zJ·K-1 <=> pK = -5.44 <=> ∆G = -52 zJ = -31.03 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 ([Fe2+]) = 0.45747 zJ·K-1 = -82.14 kJ·mol-1 \*1

πi0 ([HO2]•) = -0.18370 zJ·K-1 = 32.98 kJ·mol-1 \*1

πi0 ([Fe3+]) = 0.06676 zJ·K-1 = -11.99 kJ·mol-1 \*1

∆πi'°{[1O2] + [Fe2+] = [HO2]• + [Fe3+]} = 0.04937 zJ·K-1 <=> pK = -1.55 <=> ∆G = -15 zJ = -8.86 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 (UQ10H2) = -25.22108 zJ·K-1 = 4528.45 kJ·mol-1 \*1

πi0 (UQ10) = -25.28740 zJ·K-1 = 4540.36 kJ·mol-1 \*1

πi0 ([HO]•) = -0.37352 zJ·K-1 = 67.07 kJ·mol-1 \*2

∆πi'°{[1O2] + UQ10H2 = UQ10 + 2\*[HO]•} = -0.18959 zJ·K-1 <=> pK = 5.96 <=> ∆G = 57 zJ = 34.04 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*2

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1 \*1

πi0 ([O3]) = -0.96965 zJ·K-1 = 174.10 kJ·mol-1 \*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1 \*1

∆πi'°{2\*[1O2] + [H2O] = [O3] + [H2O2]} = -0.29663 zJ·K-1 <=> pK = 9.33 <=> ∆G = 88 zJ = 53.26 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*3

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1\*1

πi0 ([O3]) = -0.96965 zJ·K-1 = 174.10 kJ·mol-1\*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1\*1

πi0 ([3O2aq]) = -0.09134 zJ·K-1 = 16.40 kJ·mol-1\*1

∆πi'°{3\*[1O2] + [H2O] = [O3] + [H2O2] + [3O2aq]} = 0.23581 zJ·K-1 <=> pK = -7.42 <=> ∆G = -70 zJ = -42.34 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*4

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1\*1

πi0 ([O3]) = -0.96965 zJ·K-1 = 174.10 kJ·mol-1\*1

πi0 ([H2O2]) = 0.29239 zJ·K-1 = -52.50 kJ·mol-1\*1

πi0 ([3O2aq]) = -0.09134 zJ·K-1 = 16.40 kJ·mol-1\*2

∆πi'°{4\*[1O2] + [H2O] = [O3] + [H2O2] + 2\*[3O2aq]} = 0.76825 zJ·K-1 <=> pK = -24.17 <=> ∆G = -229 zJ = -137.94 kJ·mol-1

T = 298.15 K pH = 7.00 I = 0.25 M

πi0 ([1O2]) = -0.62378 zJ·K-1 = 112.00 kJ·mol-1 \*1

πi0 ([H2O]) = 0.86694 zJ·K-1 = -155.66 kJ·mol-1\*1

πi0 ([H2O3]) = -0.26618 zJ·K-1 = 47.79 kJ·mol-1\*1

∆πi'°{ [1O2] + [H2O] = [H2O3]} = -0.50934 zJ·K-1 <=> pK = 16.02 <=> ∆G = 152 zJ = 91.45 kJ·mol-1