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SUPPLEMENTARY MATERIAL TO

# Theoretical determination of the redox electrode potential of cyanidin

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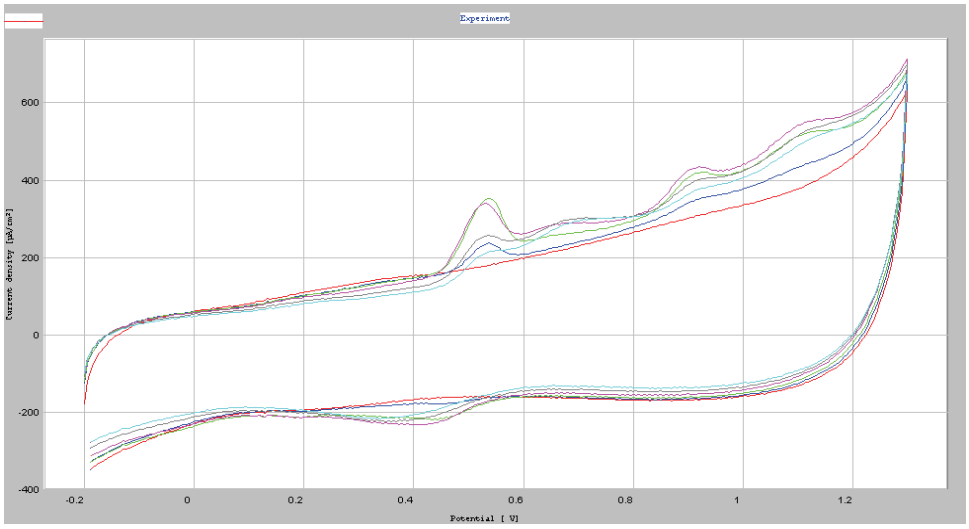


Fig. S-1. Cyclic voltammograms obtained for a methanolic solution of cyanidin.

## *Computational details*

The intermediate values that were used for the calculation of $\Delta G_T$ (see Eqs. (1)–(4) in Methodology of the native paper) and $\Delta G_{sol}$ are given in Tables S-I and S-II, respectively.

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TABLE S-I. Values of Gibbs free energies (including thermal corrections and ZPEs (Zero Point Energies)); 1 a.u. = 627.5 kcal mol$^{-1}$ (2626 kJ mol$^{-1}$); solvent = methanol

| Compound | Gas-phase energies, a.u. | Solvent energies, a.u. |
|---|---|---|
| Cy_red 1 | –1023.118992 | –1023.196070 |
| Cy_red 2 | –1023.119832 | –1023.195989 |
| Cy_red 3 | –1023.110404 | –1023.189853 |
| Cy_red 4 | –1023.109500 | –1023.189476 |
| Cy_red 5 | –1023.111252 | –1023.191810 |
| Cy_red 6 | –1023.112248 | –1023.191946 |
| Cy_ox 1 | –1021.952232 | –1022.045650 |
| Cy_ox 2 | –1021.953428 | –1022.046253 |
| Cy_ox 3 | –1021.943508 | –1022.037914 |
| Cy_ox 4 | –1021.953429 | –1022. 046253 |
| Cy_ox 5 | –1021.952232 | –1022. 045650 |
| Cy_ox 6 | –1021.953428 | –1022. 046253 |
| 1,2–Benzoquinone (Q) | –379.149551 | –379.162770 |
| 1,2–Dihydroxybenzene ($QH_2$) | –380.290650 | –380.300895 |

TABLE S-II. Solvation energies ($\Delta G_{sol}$)

| Compound | $\Delta G_{sol}$ / kcal[a] mol$^{-1}$ |
|---|---|
| Cy_red 1 | –48.37 |
| Cy_red 2 | –47.79 |
| Cy_red 3 | –49.85 |
| Cy_red 4 | –50.18 |
| Cy_red 5 | –50.55 |
| Cy_red 6 | –50.10 |
| Cy_ox 1 | –58.62 |
| Cy_ox 2 | –58.25 |
| Cy_ox 3 | –59.24 |
| Cy_ox 4 | –58.25 |
| Cy_ox 5 | –58.62 |
| Cy_ox 6 | –58.25 |
| 1,2–benzoquinone (Q) | –8.30 |
| 1,2–dihydroxybenzene (QH2) | –6.43 |

[a]1 kcal = 4184 J