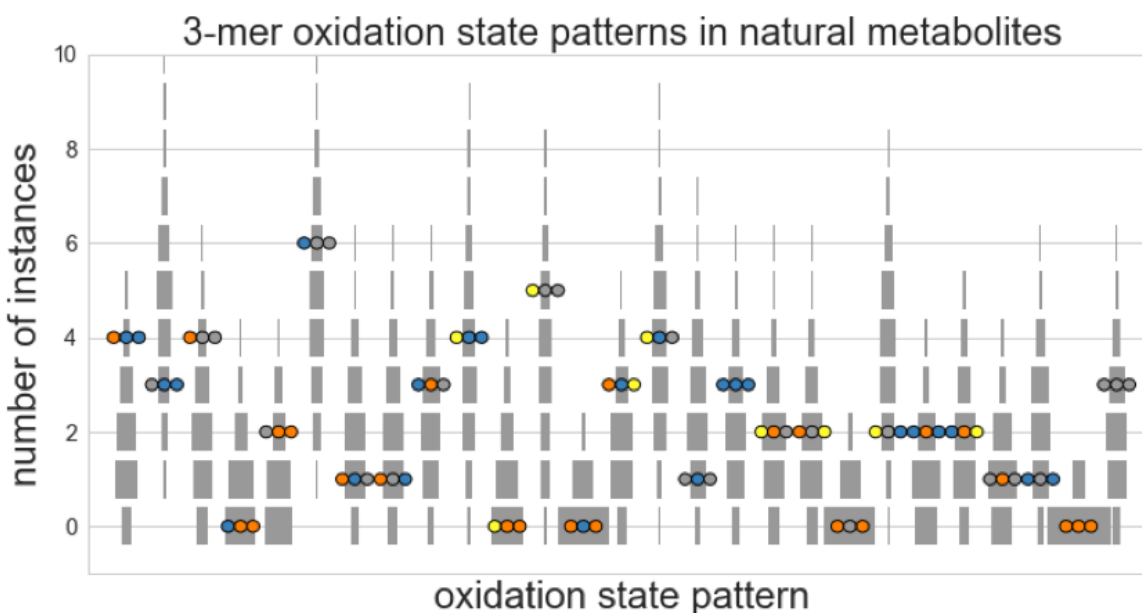
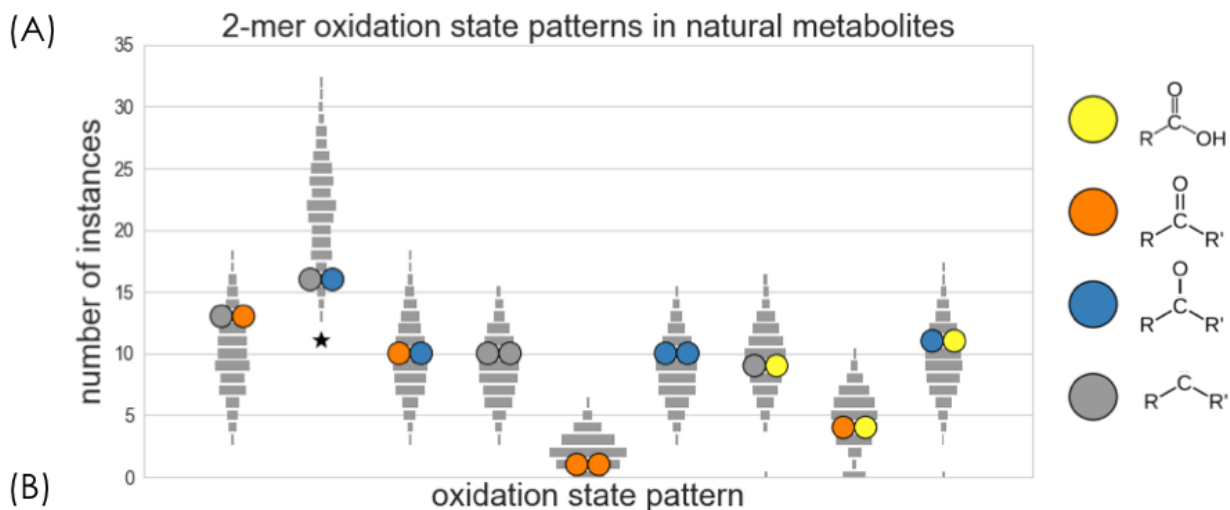
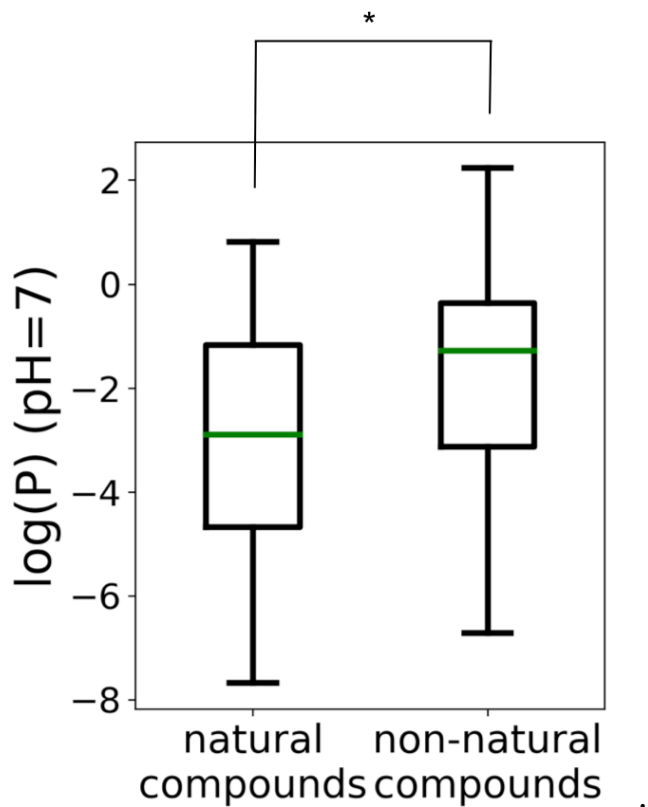


Supplementary figures for

“The thermodynamic landscape of carbon redox biochemistry”

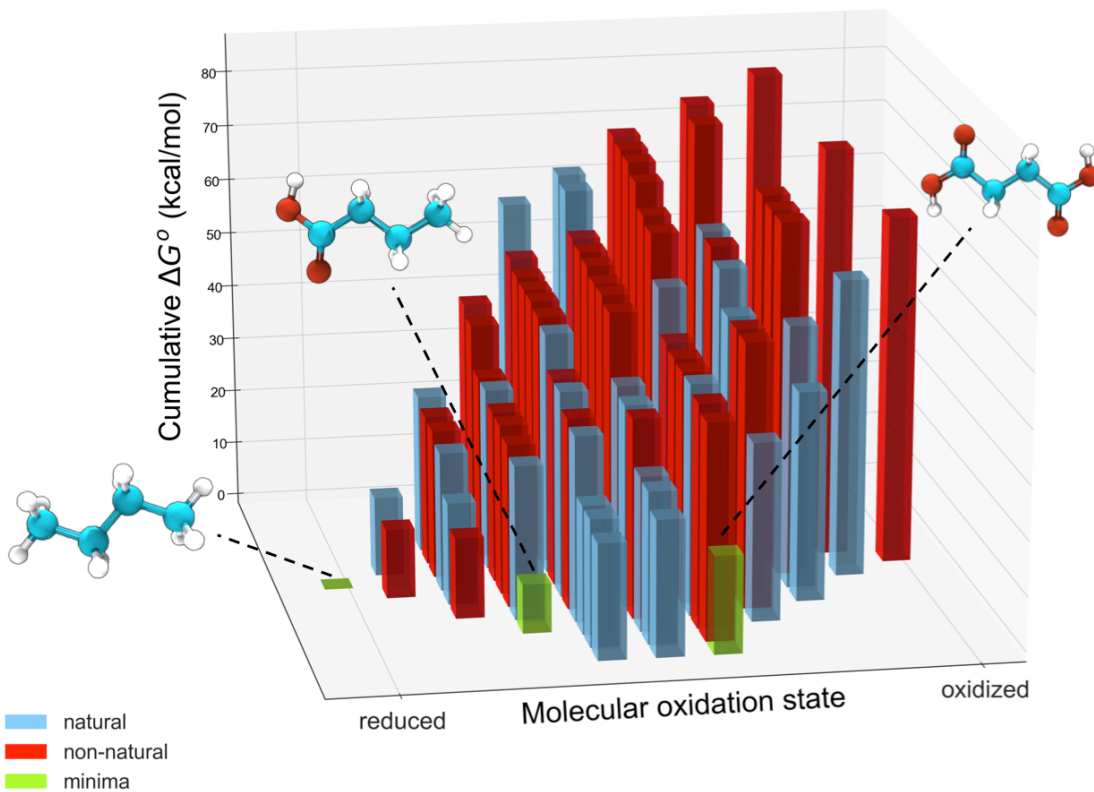


Hi wt'U3<Gptlej o gpv'cpf 'F gr rgvkqp'qhlwpevkqpcrli tqwr 'r ckt 'c'pf 'vt k rgy'r cwgt pu0a) The number of times each possible pattern of nearest neighbor functional group pairs appears in the set of natural metabolites are shown as pairs of colored circles. Gray squares correspond to the empirically-derived null distributions for randomly sampled sets of molecules from the network. The null distributions account for the single functional group (1-mer) statistics (see Methods). The pattern *hydrocarbon-alcohol* is depleted in the natural compounds, but with weak statistical significance ($p = 0.05$). b) The number of times each possible pattern of functional group triplets appears in the set of natural metabolites. No patterns are significantly enriched or depleted in the set of natural metabolites.



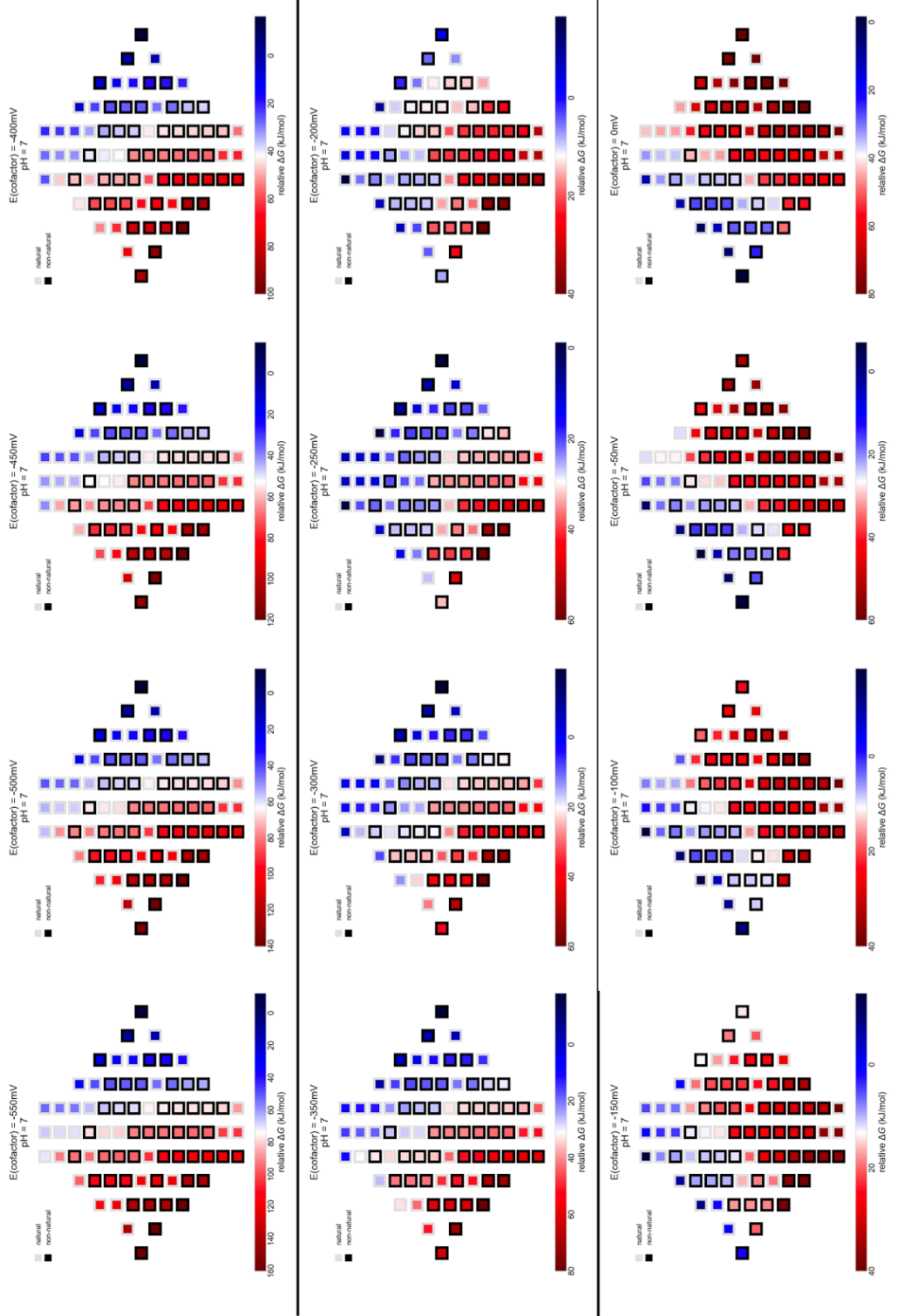
Comparison of predicted octanol-water partition coefficient $\log(P)$ at $\text{pH}=7$ for natural and non-natural compounds in the 4-carbon linear-chain redox network. This is also known as the distribution coefficient ($\log D$). Natural compounds have significantly lower $\log P(\text{pH}=7)$ than the non-natural set ($p < 0.01$).

cofactor potential = -315 mV
pH = 7



Hi wt g'U5<Vj g'5/F 't gr t gupvclqp'vj gto qf { pco le'icpf uer g'qh'vj g'6/ect dqp'hpqct 'ej clp''
t gf qz'pgvy qt ml'cv'r J ?'9'c'pf 'eqh'cevt 'r qvqp'clnG*eqh'cevt +'?'/'537'o X0Gibbs energies are
normalized relative to the metabolite with the lowest energy (butane). Thus the cumulative Gibbs
energies of a metabolite is obtained by summing up the Gibbs reaction energies of all reactions
leading to it from the reference metabolite. Compounds within a column (i.e. with the same
molecular oxidation state) are sorted according to their energies. The three compounds - butane,
butanoic acid, and succinate - which are local minima in the thermodynamic landscape are
shown. These local minima have lower energy than any of their neighboring molecules which
are accessible by either a reduction or an oxidation.

''



Hli wt g'U6<Vj gt o qf { pco k'e'icpf uecr g'qh'vj g'6/ect dqp'bgvy qt mlc'vhzgf 't J '? '9'c'pf 'xct { lpi ''
 xcnwgu'qh'G*eqhcveqt +

