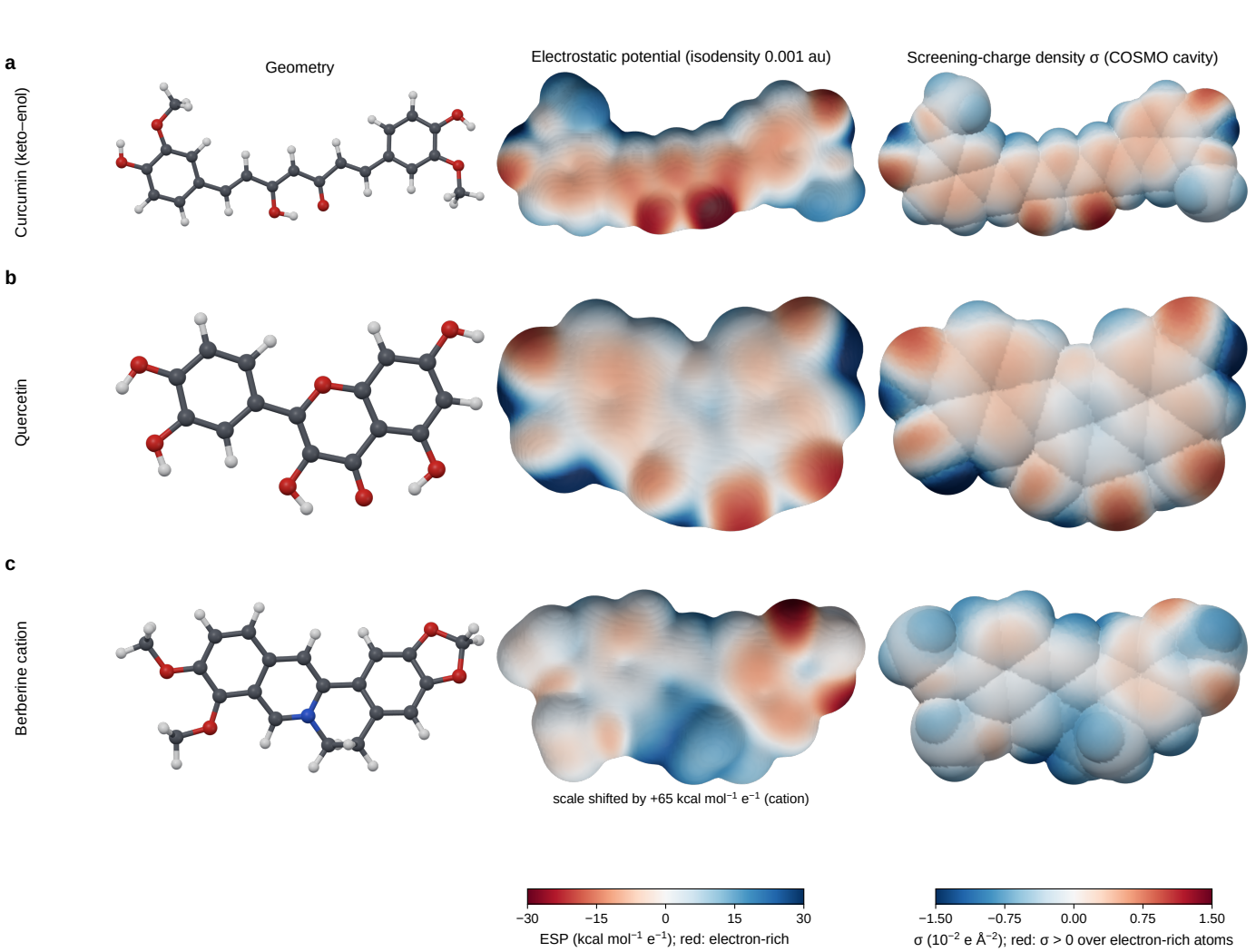

a
Curcumin (keto–enol)
Geometry
Electrostatic potential (isodensity 0.001 au)
Screening-charge density σ (COSMO cavity)
b
Quercetin
c
Berberine cation
scale shifted by +65 kcal mol⁻¹ e⁻¹ (cation)
−30
−15
0
15
30
ESP (kcal mol⁻¹ e⁻¹); red: electron-rich
−1.50
−0.75
0.00
0.75
1.50
σ (10⁻² e Å⁻²); red: σ > 0 over electron-rich atoms