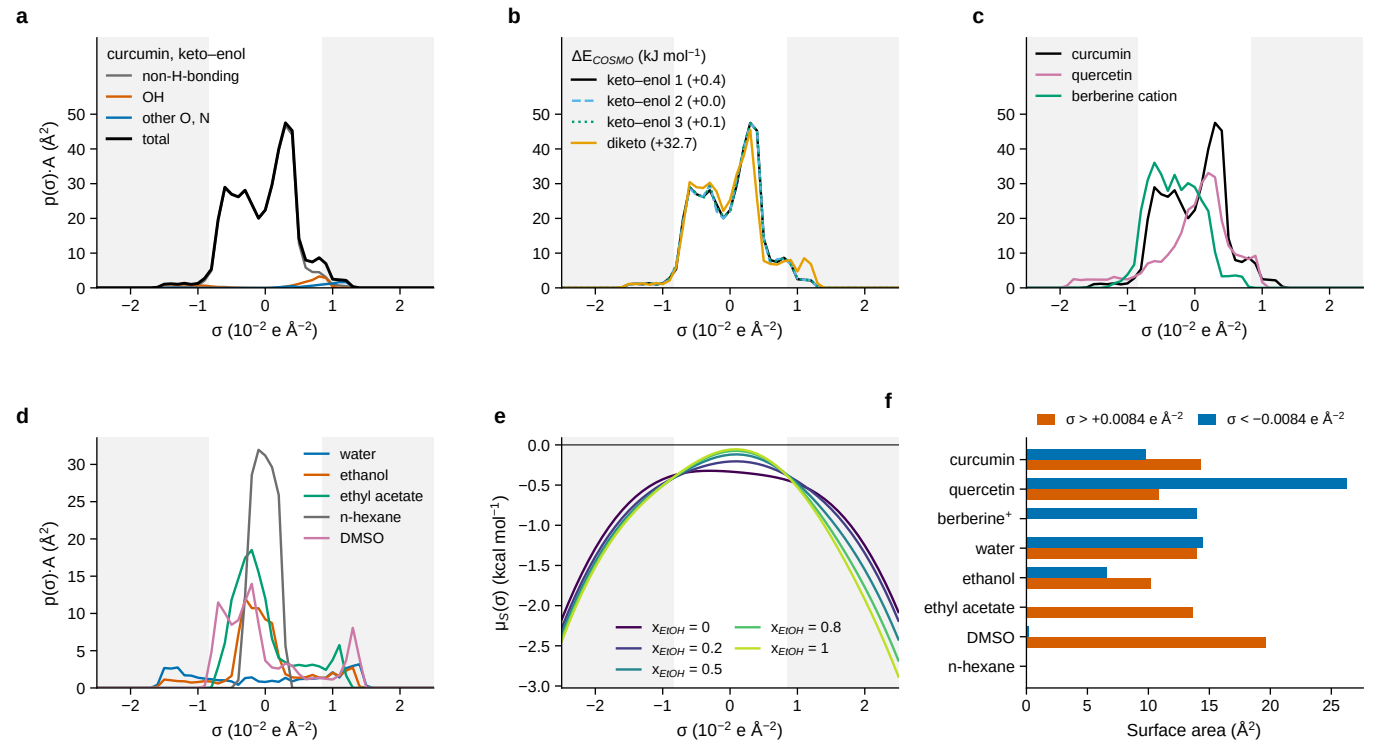

a
curcumin, keto–enol
non-H-bonding
OH
other O, N
total
p(σ)·A (Å²)
σ (10⁻² e Å⁻²)
b
ΔE_COSMO (kJ mol⁻¹)
keto–enol 1 (+0.4)
keto–enol 2 (+0.0)
keto–enol 3 (+0.1)
diketo (+32.7)
σ (10⁻² e Å⁻²)
c
curcumin
quercetin
berberine cation
σ (10⁻² e Å⁻²)
d
water
ethanol
ethyl acetate
n-hexane
DMSO
p(σ)·A (Å²)
σ (10⁻² e Å⁻²)
e
μS(σ) (kcal mol⁻¹)
xEtOH = 0
xEtOH = 0.2
xEtOH = 0.5
xEtOH = 0.8
xEtOH = 1
σ (10⁻² e Å⁻²)
f
σ > +0.0084 e Å⁻²
σ < −0.0084 e Å⁻²
curcumin
quercetin
berberine⁺
water
ethanol
ethyl acetate
DMSO
n-hexane
Surface area (Å²)