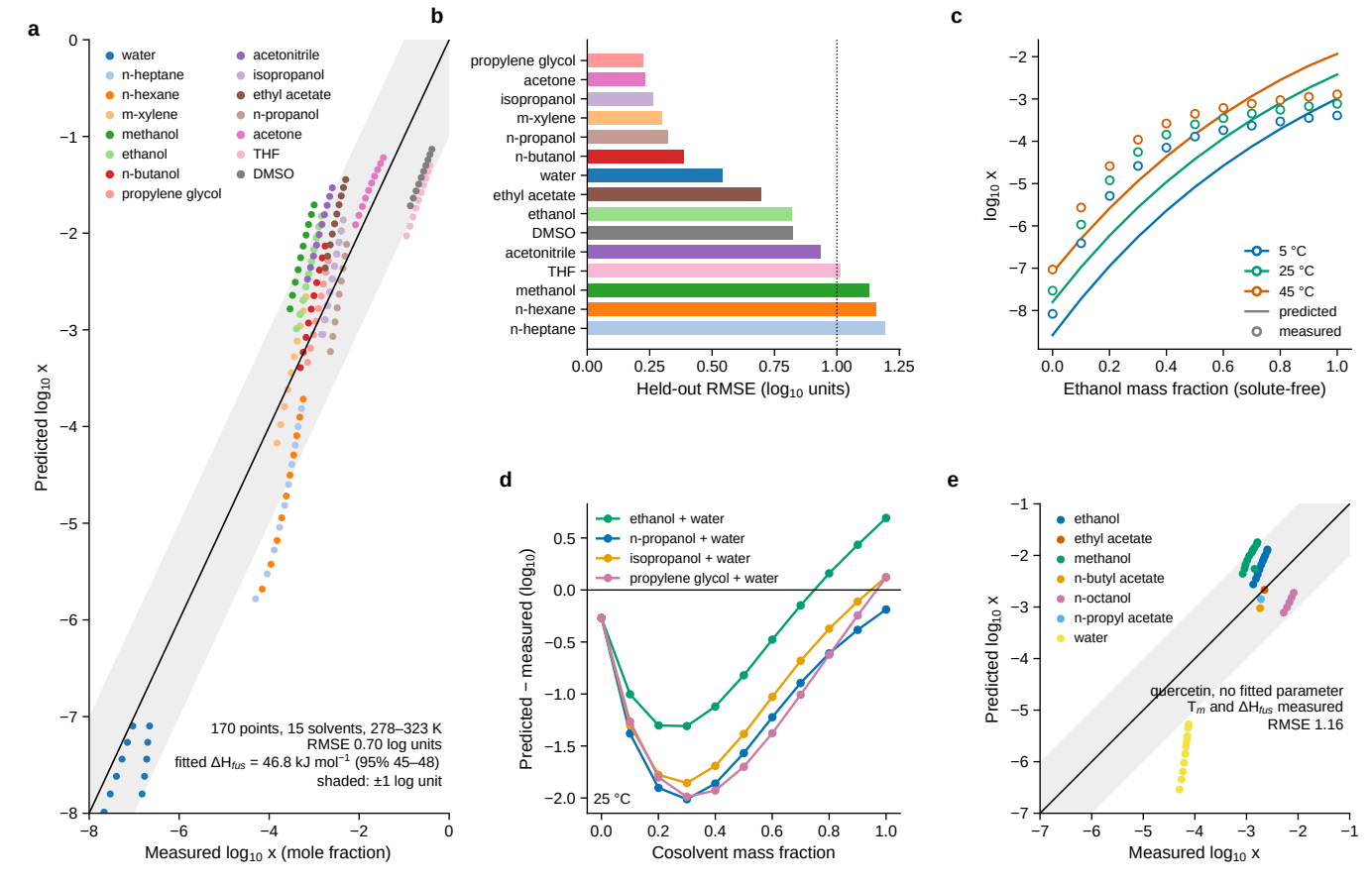

a
water
n-heptane
n-hexane
m-xylene
methanol
ethanol
n-butanol
propylene glycol
acetonitrile
isopropanol
ethyl acetate
n-propanol
acetone
THF
DMSO
170 points, 15 solvents, 278–323 K
RMSE 0.70 log units
fitted ΔH$_{fus}$ = 46.8 kJ mol^{-1} (95% 45–48)
shaded: ±1 log unit
Predicted log$_{10}$ x
Measured log$_{10}$ x (mole fraction)
b
propylene glycol
acetone
isopropanol
m-xylene
n-propanol
n-butanol
water
ethyl acetate
ethanol
DMSO
acetonitrile
THF
methanol
n-hexane
n-heptane
Held-out RMSE (log$_{10}$ units)
c
5 °C
25 °C
45 °C
predicted
measured
log$_{10}$ x
Ethanol mass fraction (solute-free)
d
ethanol + water
n-propanol + water
isopropanol + water
propylene glycol + water
25 °C
Predicted − measured (log$_{10}$)
Cosolvent mass fraction
e
ethanol
ethyl acetate
methanol
n-butyl acetate
n-octanol
n-propyl acetate
water
quercetin, no fitted parameter
T$_m$ and ΔH$_{fus}$ measured
RMSE 1.16
Predicted log$_{10}$ x
Measured log$_{10}$ x