Supporting Information

Molecular Innovations in Nanofiltration via Interfacial Polymerization: From Monomer Design to Membrane Performance

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Text S1 Solute/solute selectivity[1]:

The separation factor (S) of solute A to solute B is a typical adopted parameter to characterize solute/solute selectivity in a membrane separation process, and can be calculated using the following equation:

$$S = \frac{1 - R_A}{1 - R_B}$$

Where R_A represents the solvent rejection rate of A and R_B represents the solvent rejection rate of B.
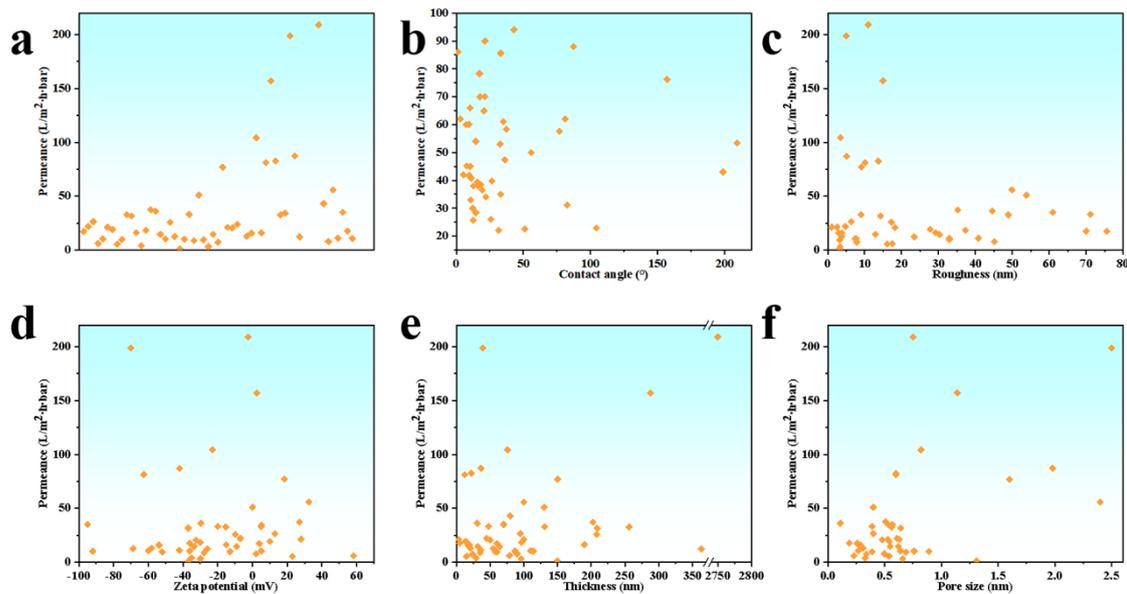
Fig. S1 (a) Permeances of novel monomer-based NF membranes. Their permeances as a function of (b) contact angle, (c) surface roughness, (d) surface potential, (e) active layer thickness, and (f) pore size.
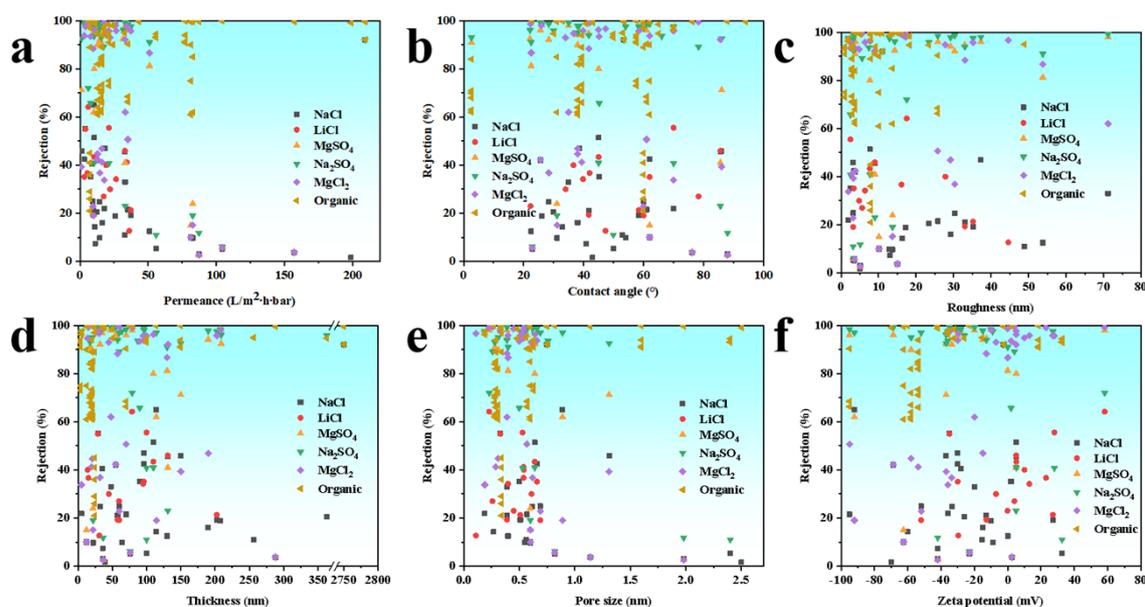

Fig. S2 (a) Correlation between the permeances of novel monomer-based NF membranes and the rejection rates of monovalent salts, divalent salts, and organic compounds. Their rejection rates as a function of (b) contact angle, (c) surface roughness, (d) active layer thickness, (e) pore size, and (f) surface potential.
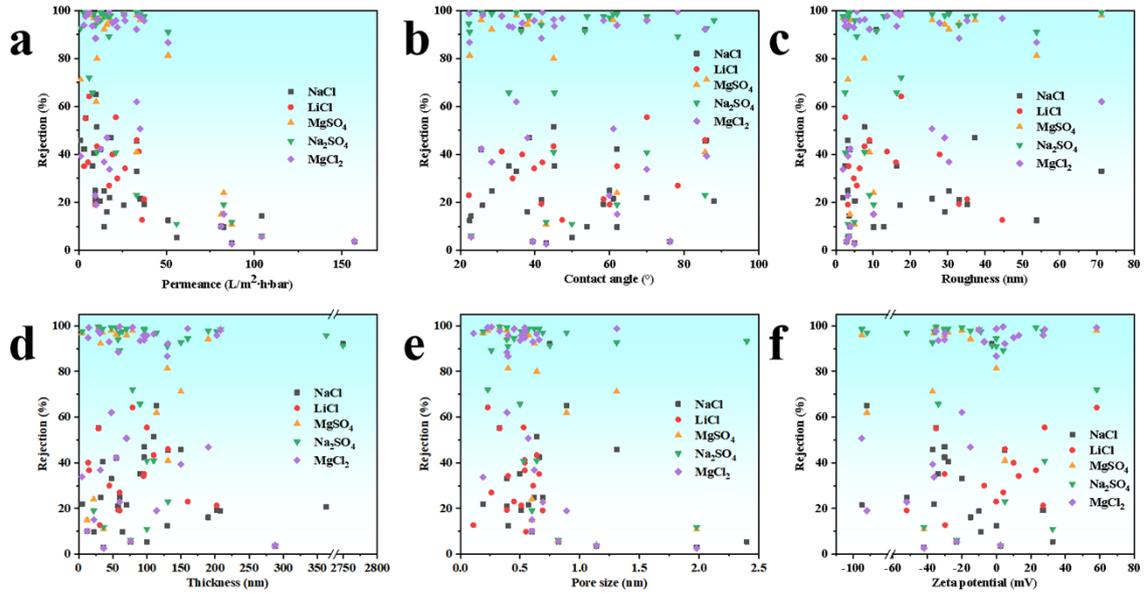
Fig. S3 (a) Correlation between permeances and rejection rates of monovalent/divalent salts. The rejection rates of monovalent/divalent salts as a function of (b) contact angle, (c) surface roughness, (d) active layer thickness, (e) pore size, and (f) surface potential.
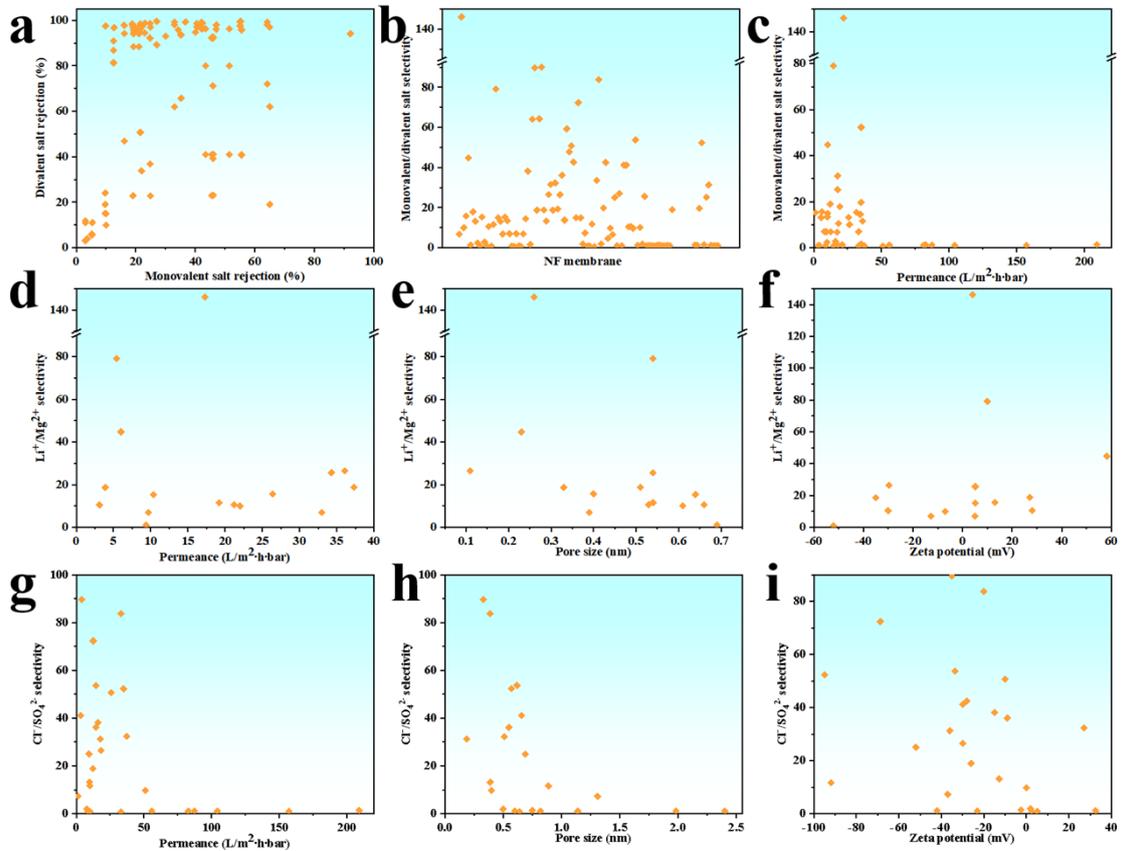

Fig. S4 (a) Correlation of rejection rates between monovalent and divalent salts. (b) Separation factors for monovalent/divalent salts. (c) Correlation between permeances

and separation factors of monovalent/divalent salts. The Li^+/Mg^{2+} selectivity as a function of (d) permeance, (e) pore size, and (f) surface potential. The Cl^-/SO_4^{2-} selectivity as a function of (g) permeance, (h) pore size, and (i) surface potential.
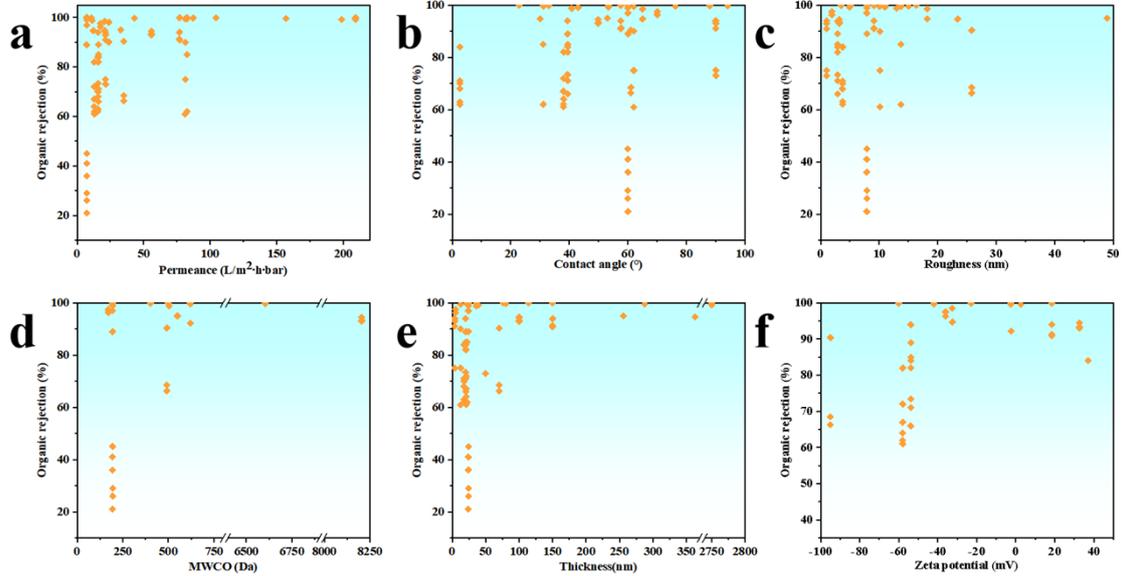

Fig. S5 (a) Correlation between permeances and rejection rates of organic compounds. The rejection rates of organic compounds as a function of (b) contact angle, (c) surface roughness, (d) molecular weight cut-off (MWCO), (e) active layer thickness, and (f) surface potential.
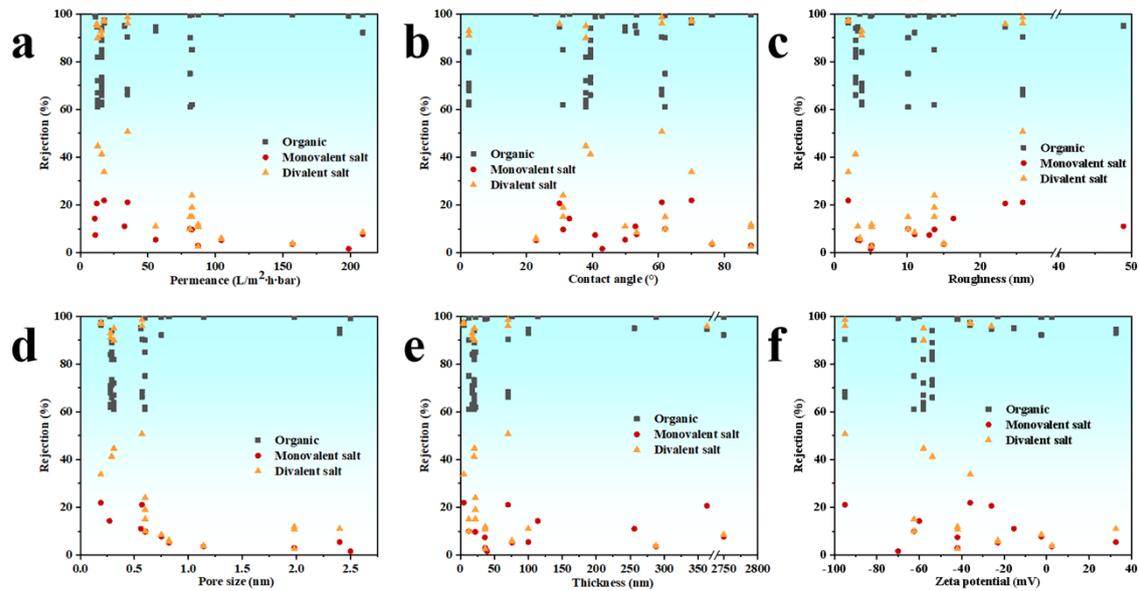

Fig. S6 (a) Correlation between permeances and rejection rates of salts and organic compounds. The rejection rates of salts and organic compounds as a function of (b) contact angle, (c) surface roughness, (d) pore size, and (e) active layer thickness.
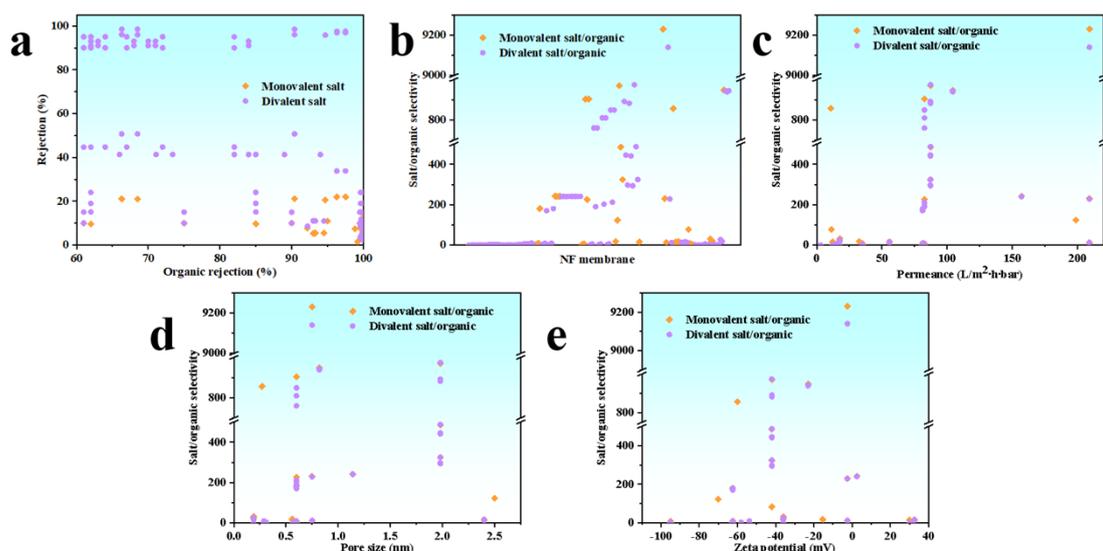
Fig. S7 (a) Correlation among the rejection rates of monovalent salts, divalent salts, and organic compounds. (b) Separation factors of membranes for monovalent salts/organic compounds and divalent salts/organic compounds. Their separation factors as a function of (c) permeance, (d) pore size, and (e) surface potential.

Table S1 Comparison of cost and performance for commercial versus laboratory-scale NF membranes

	Commercial	Laboratory-scale NF
Raw material cost	1 ~ 3 $/m²	20 ~ 300 $/m²
Synthesis cost	3 ~ 6 $/m²	30 ~ 500 $/m²
Batch production cost	15 ~ 25 $/m²	Nearly impossible
Wastewater treatment cost	0.5 ~ 1.5 $/m²	Seldom
Permeance	3 ~ 10 L/m²·h·bar	1 ~ 210 L/m²·h·bar
Salt selectivity	2 ~ 8	1 ~ 190
Long-term stability	2 ~ 5 years	1 ~ 12 days

Note: Costs are influenced by multiple factors, including raw material prices, production scale, and manufacturer-specific conditions, resulting in variability across different suppliers and production scenarios.

References

1. K. Wang, X. Wang, B. Januszewski, Y. Liu, D. Li, R. Fu, M. Elimelech and X. Huang, *Chemical Society Reviews*, 2022, **51**, 672-719.