Supporting Information

Emerging investigators series: Post -Synthesis Modification of Reverse Osmosis Membranes for the Enhanced Separation of Small Neutral Molecules

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Calibration curve for NaCl solution and Urea solution

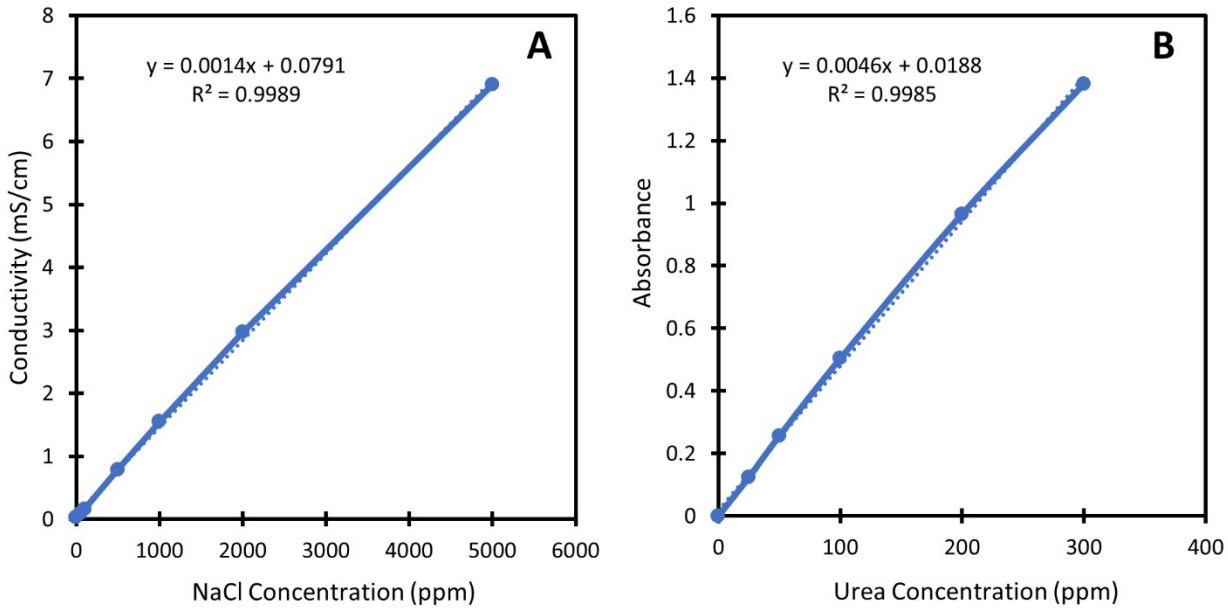

Figure S1. Calibration curve for (A) NaCl solutions and (B) urea solutions in water.

FTIR data (1200 cm^{-1} - 1800 cm^{-1} range) for XLE membranes modified using amines in post modification

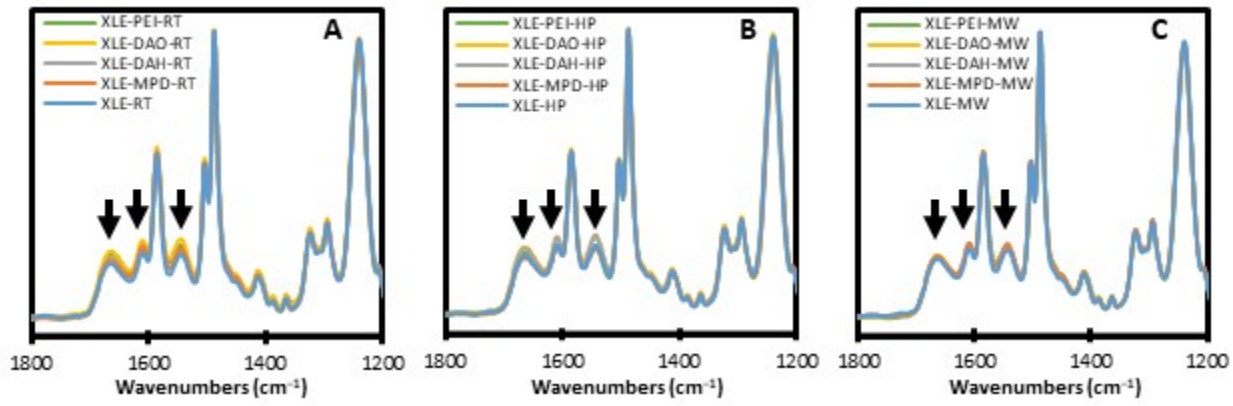

Figure S2. ATR-FTIR spectra of (A) XLE membranes modified with/without amines at room temperature, (B) XLE membranes modified with/without amines and then heat treated with the hot plate, and (C) XLE membranes modified with/without amines and then heat treated with the microwave oven.

SEM data for XLE membranes modified using amines in post modification

The control and modified XLE membrane surface morphology was studied using an Apreo field emission scanning electron microscope (FE-SEM, Thermo Fisher Scientific). The membrane samples were dried, attached with carbon tape to aluminum stabs, and sputter-coated with ~12 nm of gold (MCM-200 ion sputter coater, SEC Co., Ltd., Korea) prior to SEM imaging. The SEM images were taken at an accelerating voltage of 5 kV, a current voltage of 50 pA, and a magnification of 10,000x.

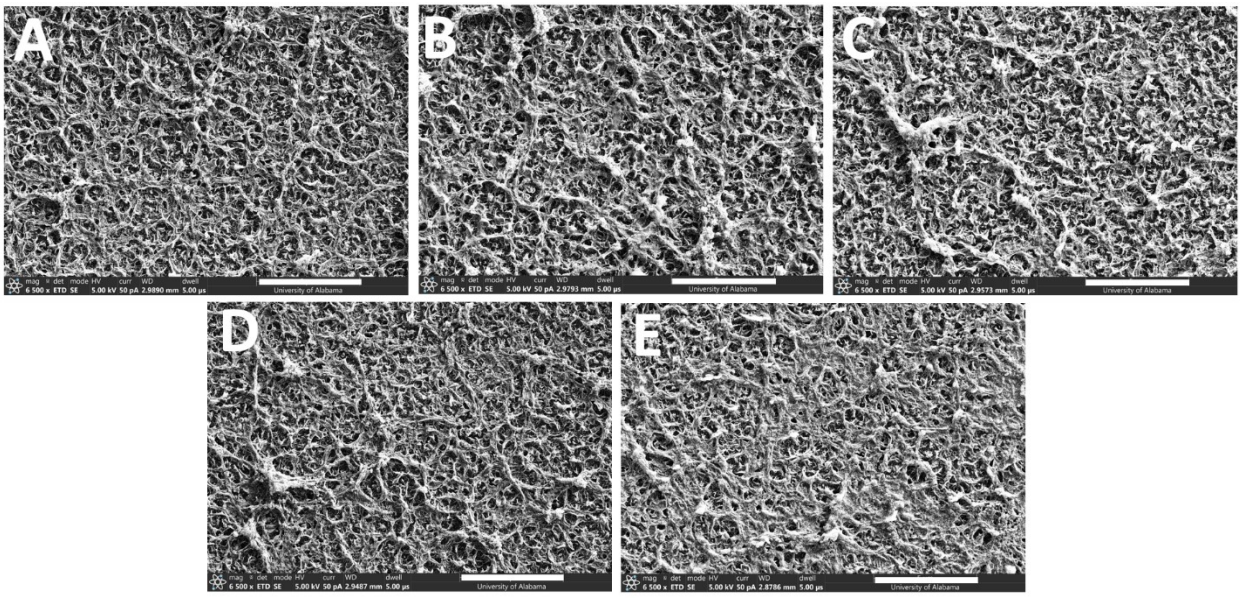

Figure S3. SEM images of (A) XLE-RT, (B) XLE-DAH-RT, (C) XLE-DAO-RT, (D) XLE-MPD-RT, and (E) XLE-PEI-RT membranes. The white scale bar represents 5 μm.

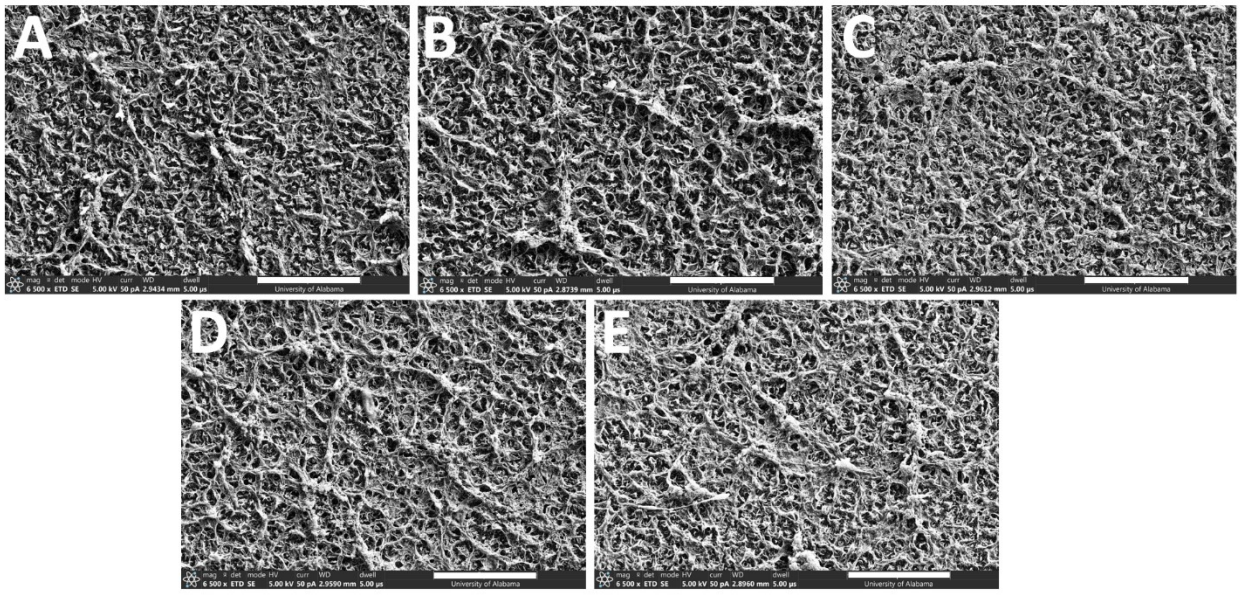

Figure S4. SEM images of (A) XLE-HP, (B) XLE-DAH-HP, (C) XLE-DAO-HP, (D) XLE-MPD-HP, and (E) XLE-PEI-HP membranes. The white scale bar represents 5 μm.

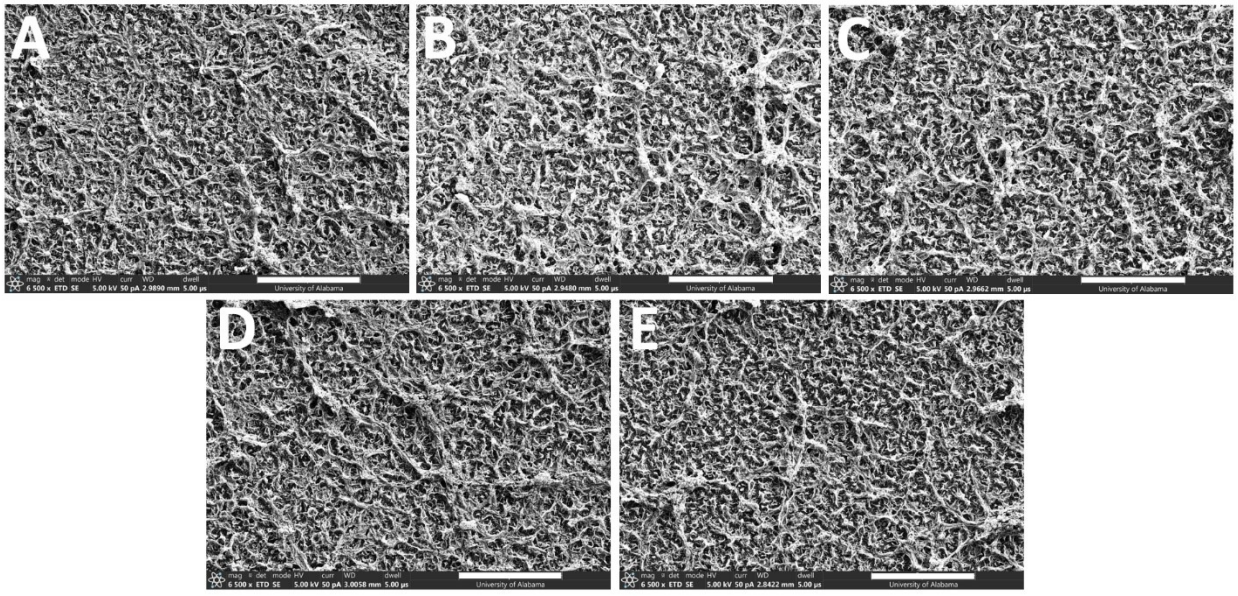

Figure S5. SEM images of (A) XLE-MW, (B) XLE-DAH-MW, (C) XLE-DAO-MW, (D) XLE-MPD-MW, and (E) XLE-PEI-MW membranes. The white scale bar represents 5 μm.

Results of Paired t-tests

Results from Paired Two sample t-test for Means Hypothesis testing was done to determine statistical relevance of the data sets. EXCEL (Microsoft O365 Version 1908) was used for all statistical analyses. All tests were done using 95% confidence ($\alpha = 0.05$); therefore, if the p-value is greater than α then the means are considered to be equal and if the p-value is less than α then the means are considered to be unequal. **Table S1** shows the results from the statistical tests on the contact angle from **Figure 3** in the main document. **Table S2** and **Table S3** show the results from the statistical tests on the pure water permeance and NaCl rejection data from **Figures 4A, 4B, and 4C** in the main document for the 2,000 ppm NaCl feed. **Table S4** shows the results from the statistical tests on the urea rejection data from **Figure 5** in the main document for the 500 ppm urea feed. **Table S5** shows the results from the statistical tests on the boron rejection data from **Figure 6** in the main document for the 40 ppm boric acid feed.

Table S1. Results of paired t-tests on pure water permeance.

Group 1 Data	Group 2 Data	Data	Two-tailed P value	Result of Difference
XLE-RT	XLE-DAH-RT	Pure Water Permeance	0.0232	Statistically significant
XLE-RT	XLE-DAO-RT	Pure Water Permeance	0.0000	Statistically significant
XLE-RT	XLE-MPD-RT	Pure Water Permeance	0.0005	Statistically significant
XLE-RT	XLE-PEI-RT	Pure Water Permeance	0.0006	Statistically significant
XLE-HP	XLE-DAH-HP	Pure Water Permeance	0.0043	Statistically significant
XLE-HP	XLE-DAO-HP	Pure Water Permeance	0.0002	Statistically significant
XLE-HP	XLE-MPD-HP	Pure Water Permeance	0.0045	Statistically significant
XLE-HP	XLE-PEI-HP	Pure Water Permeance	0.0036	Statistically significant
XLE-MW	XLE-DAH-MW	Pure Water Permeance	0.5432	Not statistically significant
XLE-MW	XLE-DAO-MW	Pure Water Permeance	0.0051	Statistically significant
XLE-MW	XLE-MPD-MW	Pure Water Permeance	0.6928	Not statistically significant
XLE-MW	XLE-PEI-MW	Pure Water Permeance	0.3020	Not statistically significant
XLE-DAH-HP	XLE-DAH-MW	Pure Water Permeance	0.2805	Not statistically significant
XLE-DAH-RT	XLE-DAH-MW	Pure Water Permeance	0.0046	Statistically significant
XLE-DAH-RT	XLE-DAH-HP	Pure Water Permeance	0.0048	Statistically significant
XLE-DAO-HP	XLE-DAO-MW	Pure Water Permeance	0.1943	Not statistically significant
XLE-DAO-RT	XLE-DAO-MW	Pure Water Permeance	0.1499	Statistically significant

XLE-DAO-RT	XLE-DAO-HP	Pure Water Permeance	0.0105	Not statistically significant
XLE-MPD-HP	XLE-MPD-MW	Pure Water Permeance	0.1274	Not statistically significant
XLE-MPD-RT	XLE-MPD-MW	Pure Water Permeance	0.0086	Statistically significant
XLE-MPD-RT	XLE-MPD-HP	Pure Water Permeance	0.0165	Not statistically significant
XLE-PEI-HP	XLE-PEI-MW	Pure Water Permeance	0.4252	Not statistically significant
XLE-PEI-RT	XLE-PEI-MW	Pure Water Permeance	0.0219	Statistically significant
XLE-PEI-RT	XLE-PEI-HP	Pure Water Permeance	0.0743	Not statistically significant
XLE-RT	XLE-MW	Pure Water Permeance	0.0002	Statistically significant
XLE-RT	XLE-HP	Pure Water Permeance	0.0081	Statistically significant
XLE-HP	XLE-MW	Pure Water Permeance	0.0109	Statistically significant

Table S2. Results of paired t-tests on NaCl rejection.

Group 1 Data	Group 2 Data	Data	Two-tailed P value	Result of Difference
XLE-RT	XLE-DAH-RT	NaCl Rejection	0.6067	Not statistically significant
XLE-RT	XLE-DAO-RT	NaCl Rejection	0.0145	Statistically significant
XLE-RT	XLE-MPD-RT	NaCl Rejection	0.7274	Not statistically significant
XLE-RT	XLE-PEI-RT	NaCl Rejection	0.2442	Not statistically significant
XLE-HP	XLE-DAH-HP	NaCl Rejection	0.1662	Not statistically significant
XLE-HP	XLE-DAO-HP	NaCl Rejection	0.3582	Not statistically significant

XLE-HP	XLE-MPD-HP	NaCl Rejection	0.7392	Not statistically significant
XLE-HP	XLE-PEI-HP	NaCl Rejection	0.2135	Not statistically significant
XLE-MW	XLE-DAH-MW	NaCl Rejection	0.5852	Not statistically significant
XLE-MW	XLE-DAO-MW	NaCl Rejection	0.4429	Not statistically significant
XLE-MW	XLE-MPD-MW	NaCl Rejection	0.1246	Not statistically significant
XLE-MW	XLE-PEI-MW	NaCl Rejection	0.3394	Not statistically significant
XLE-DAH-HP	XLE-DAH-MW	NaCl Rejection	0.1392	Not statistically significant
XLE-DAH-RT	XLE-DAH-MW	NaCl Rejection	0.8024	Not statistically significant
XLE-DAH-RT	XLE-DAH-HP	NaCl Rejection	0.2104	Not statistically significant
XLE-DAO-HP	XLE-DAO-MW	NaCl Rejection	0.1498	Not statistically significant
XLE-DAO-RT	XLE-DAO-MW	NaCl Rejection	0.0079	Statistically significant
XLE-DAO-RT	XLE-DAO-HP	NaCl Rejection	0.1816	Not statistically significant
XLE-MPD-HP	XLE-MPD-MW	NaCl Rejection	0.1833	Not statistically significant
XLE-MPD-RT	XLE-MPD-MW	NaCl Rejection	0.0495	Statistically significant
XLE-MPD-RT	XLE-MPD-HP	NaCl Rejection	0.8884	Not statistically significant
XLE-PEI-HP	XLE-PEI-MW	NaCl Rejection	0.4756	Not statistically significant
XLE-PEI-RT	XLE-PEI-MW	NaCl Rejection	0.5417	Not statistically significant
XLE-PEI-RT	XLE-PEI-HP	NaCl Rejection	0.8227	Not statistically significant

XLE-RT	XLE-MW	NaCl Rejection	0.7907	Not statistically significant
XLE-RT	XLE-HP	NaCl Rejection	0.6952	Not statistically significant
XLE-HP	XLE-MW	NaCl Rejection	0.8626	Not statistically significant

Table S3. Results of paired t-tests on urea rejection.

Group 1 Data	Group 2 Data	Data	Two-tailed P value	Result of Difference
XLE-RT	XLE-DAH-RT	Urea Rejection	0.0143	Statistically significant
XLE-RT	XLE-DAO-RT	Urea Rejection	0.0000	Statistically significant
XLE-RT	XLE-MPD-RT	Urea Rejection	0.0060	Statistically significant
XLE-RT	XLE-PEI-RT	Urea Rejection	0.0040	Statistically significant
XLE-HP	XLE-DAH-HP	Urea Rejection	0.0075	Statistically significant
XLE-HP	XLE-DAO-HP	Urea Rejection	0.0010	Statistically significant
XLE-HP	XLE-MPD-HP	Urea Rejection	0.0106	Statistically significant
XLE-HP	XLE-PEI-HP	Urea Rejection	0.7750	Not statistically significant
XLE-MW	XLE-DAH-MW	Urea Rejection	0.0034	Statistically significant
XLE-MW	XLE-DAO-MW	Urea Rejection	0.0009	Statistically significant
XLE-MW	XLE-MPD-MW	Urea Rejection	0.0001	Statistically significant
XLE-MW	XLE-PEI-MW	Urea Rejection	0.0374	Statistically significant
XLE-DAH-HP	XLE-DAH-MW	Urea Rejection	0.7339	Not statistically significant

XLE-DAH-RT	XLE-DAH-MW	Urea Rejection	0.0028	Statistically significant
XLE-DAH-RT	XLE-DAH-HP	Urea Rejection	0.0015	Statistically significant
XLE-DAO-HP	XLE-DAO-MW	Urea Rejection	0.9818	Not statistically significant
XLE-DAO-RT	XLE-DAO-MW	Urea Rejection	0.0216	Statistically significant
XLE-DAO-RT	XLE-DAO-HP	Urea Rejection	0.0009	Statistically significant
XLE-MPD-HP	XLE-MPD-MW	Urea Rejection	0.0675	Not statistically significant
XLE-MPD-RT	XLE-MPD-MW	Urea Rejection	0.0019	Statistically significant
XLE-MPD-RT	XLE-MPD-HP	Urea Rejection	0.0018	Statistically significant
XLE-PEI-HP	XLE-PEI-MW	Urea Rejection	0.8112	Not statistically significant
XLE-PEI-RT	XLE-PEI-MW	Urea Rejection	0.0000	Statistically significant
XLE-PEI-RT	XLE-PEI-HP	Urea Rejection	0.0070	Statistically significant
XLE-RT	XLE-MW	Urea Rejection	0.0000	Statistically significant
XLE-RT	XLE-HP	Urea Rejection	0.0002	Statistically significant
XLE-HP	XLE-MW	Urea Rejection	0.8161	Not statistically significant

Table S4. Results of paired t-tests on boron rejection.

Group 1 Data	Group 2 Data	Data	Two-tailed P value	Result of Difference
XLE-RT	XLE-DAH-HP	Boron Rejection	0.0003	Statistically significant
XLE-RT	XLE-DAO-HP	Boron Rejection	0.0031	Statistically significant

XLE-RT	XLE-MPD-HP	Boron Rejection	0.0002	Statistically significant
XLE-RT	XLE-PEI-HP	Boron Rejection	0.0428	Statistically significant
XLE-RT	XLE-HP	Boron Rejection	0.0034	Statistically significant

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65 **Table S5.** Results of paired t-tests on water contact angle measurement.

Group 1 Data	Group 2 Data	Data	Two-tailed P value	Result of Difference
XLE-RT	XLE-DAH-RT	Contact Angle	0.0000	Statistically significant
XLE-RT	XLE-DAO-RT	Contact Angle	0.0009	Statistically significant
XLE-RT	XLE-MPD-RT	Contact Angle	0.0000	Statistically significant
XLE-RT	XLE-PEI-RT	Contact Angle	0.0008	Statistically significant
XLE-HP	XLE-DAH-HP	Contact Angle	0.0000	Statistically significant
XLE-HP	XLE-DAO-HP	Contact Angle	0.0000	Statistically significant
XLE-HP	XLE-MPD-HP	Contact Angle	0.0002	Statistically significant
XLE-HP	XLE-PEI-HP	Contact Angle	0.0259	Statistically significant
XLE-MW	XLE-DAH-MW	Contact Angle	0.0000	Statistically significant
XLE-MW	XLE-DAO-MW	Contact Angle	0.0000	Statistically significant
XLE-MW	XLE-MPD-MW	Contact Angle	0.0000	Statistically significant
XLE-MW	XLE-PEI-MW	Contact Angle	0.0003	Statistically significant
XLE-DAH-HP	XLE-DAH-MW	Contact Angle	0.3190	Not statistically significant

XLE-DAH-RT	XLE-DAH-MW	Contact Angle	0.0014	Statistically significant
XLE-DAH-RT	XLE-DAH-HP	Contact Angle	0.0009	Statistically significant
XLE-DAO-HP	XLE-DAO-MW	Contact Angle	0.0382	Statistically significant
XLE-DAO-RT	XLE-DAO-MW	Contact Angle	0.0025	Statistically significant
XLE-DAO-RT	XLE-DAO-HP	Contact Angle	0.1616	Not statistically significant
XLE-MPD-HP	XLE-MPD-MW	Contact Angle	0.3610	Not statistically significant
XLE-MPD-RT	XLE-MPD-MW	Contact Angle	0.0654	Not statistically significant
XLE-MPD-RT	XLE-MPD-HP	Contact Angle	0.0240	Statistically significant
XLE-PEI-HP	XLE-PEI-MW	Contact Angle	0.8634	Not statistically significant
XLE-PEI-RT	XLE-PEI-MW	Contact Angle	0.0726	Not statistically significant
XLE-PEI-RT	XLE-PEI-HP	Contact Angle	0.1938	Not statistically significant
XLE-RT	XLE-MW	Contact Angle	0.1653	Not statistically significant
XLE-RT	XLE-HP	Contact Angle	0.0102	Statistically significant
XLE-HP	XLE-MW	Contact Angle	0.1607	Not statistically significant

Minimal projection area, pK_as, and Octanol water partition coefficient data of amines used in modified XLE membranes

Table S6. Minimal projection area, pK_as, and Octanol water partition coefficient data of MPD, DAH, DAO and PEI from http://www.chemicalize.org website.)

Compound	pK_{a1}	pK_{a2}	Octanol water Coefficient
MPD	2.73	5.48	0.315
DAH	9.90	10.51	0.044
DAO	9.90	10.51	0.933
PEI	10.16	------	-0.279
Urea	------	------	-1.364
Boric Acid	8.70	12.11	-0.509