Supplementary File of: Machine-Learning-Assisted Low Dielectric Constant Polymer Discovery

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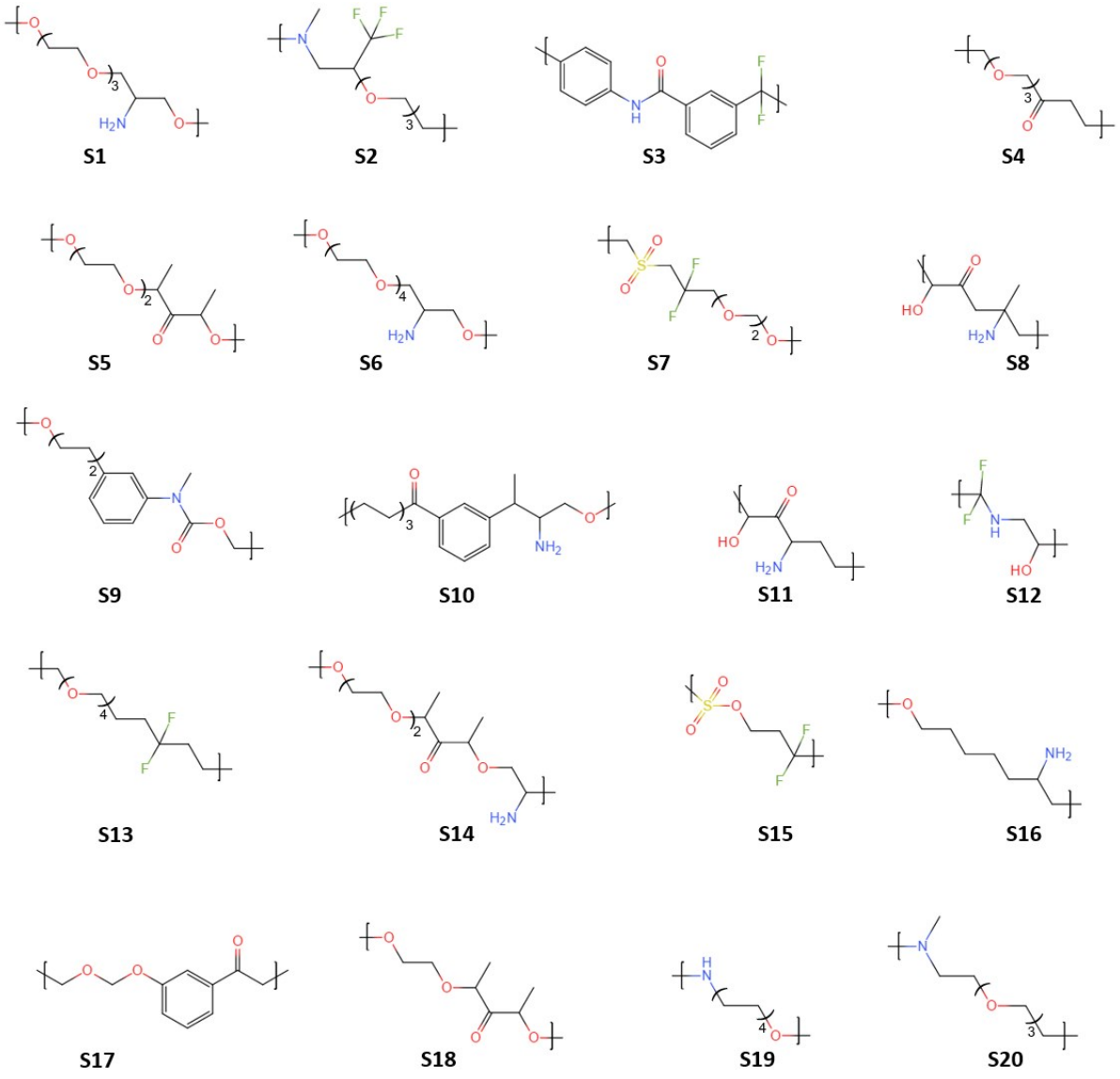
Section 1. More predicted polymers with low dielectric constant

From the Decision Tree generated by Random Forest, we can predict more polymers based on different functional group combinations and number of each group. In this Figure S1, we present twenty different low dielectric constant polymer that are all different from the twenty polymers in the main text.

Figure S1. Predicted polymers with low dielectric constant.



Section 2. Synthesis route of p-ADMHOTC, p-ATOTD and p-DMHOND and result of p-ADMHOTC

Synthesis of 20-amino-15,17-dimethyl-2,5,8,11,14,18,22-heptaoxatricosan-16-one (p-ADMHOTC)

Dissolve 2 mmol TEG, 2 mmol 2-amino-1, 3-propanediol, 8 mmol TEA, and 2mmol DMAP in 40ml dry $CHCl_3$ in a three-neck round-bottom flask. Cool the solution in an ice-water bath to 0^{o}C and add 4mmol 2,4-dibromo-3-pentanone (dissolve in 10ml dry $CHCl_3$ in advance) dropwise in 1h under dry N_2. After 48h reaction at room

temperature, the reaction solution was repeatedly extracted with water/CH_2Cl_2, and the product dissolved in the aqueous phase. The process is shown in Figure S2 (a).

Synthesis of 11-amino-2,6,9,13-tetraoxatetradecan-4-ol (p-ATOTD)

Dissolve 2 mmol propane-1,2,3-triol, 2 mmol 2-amino-1, 3-propanediol, 8 mmol TEA and 2mmol DMAP in 40ml dry $CHCl_3$ in a three-neck round-bottom flask. Cool the solution in an ice-water bath to 0°C and add 4mmol 1,2-dibromoethane (dissolve in 10ml dry $CHCl_3$ in advance) dropwise in 1h under dry N_2. After 48h reaction at room temperature, the reaction solution was repeatedly extracted with water/CH_2Cl_2, and the product dissolved in the aqueous phase. The process is shown in Figure S2 (b).

Synthesis of 15,17-dimethyl-2,5,8,11,14,18-hexaoxanonadecan-16-one (p-

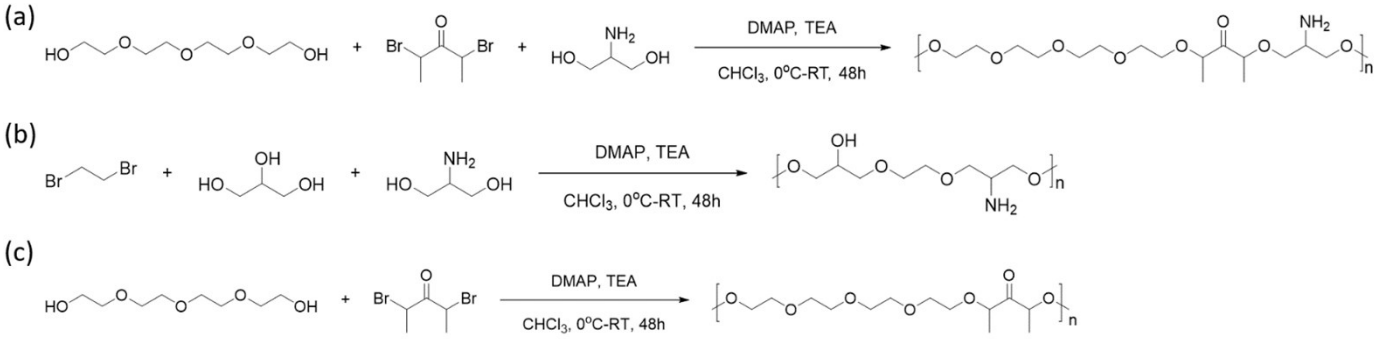


Figure S2. Synthetic routs for (a) 20-amino-15,17-dimethyl-2,5,8,11,14,18,22-heptaoxatricosan-16-one (p-ADMHOTC), (b) 11-amino-2,6,9,13-tetraoxatetradecan-4-ol (p-ATOTD), and (c) 15,17-dimethyl-2,5,8,11,14,18-hexaoxanonadecan-16-one (p-DMHOND).

DMHOND)

Dissolve 2 mmol TEG, 8 mmol TEA, and 2mmol DMAP in 40ml dry $CHCl_3$ in a three-neck round-bottom flask. Cool the solution in an ice-water bath to 0oC and add 4mmol 2,4-dibromo-3-pentanone (dissolve in 10ml dry $CHCl_3$ in advance) dropwise in 1h under dry N_2. After 48h reaction at room temperature, the reaction solution was repeatedly extracted with water/CH_2Cl_2, and the product dissolved in the aqueous phase. The process is shown in Figure S2 (c).

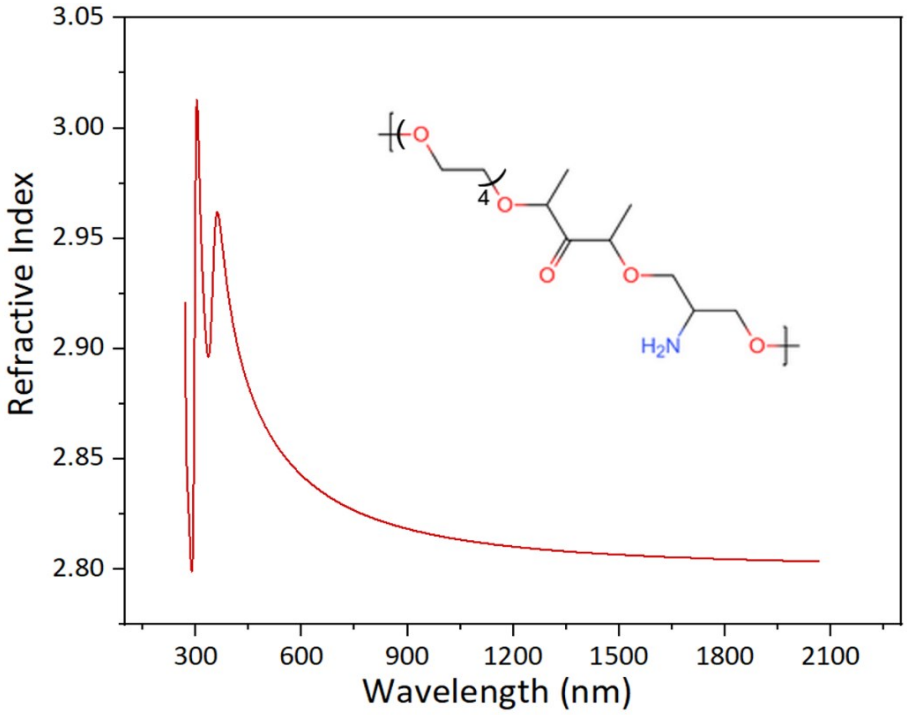


Figure S3. Testing result of predicted polymer p-ADMHOTC. The n is about 2.80-3.01, and the ε_0 is 7.85.