

# polySML: structure & machine learning for polymer materials

This suite of standalone software is to predict mechanical, thermal, conductivity, filtration and separational etc. properties for variant polymer materials.

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## 1 Requirements

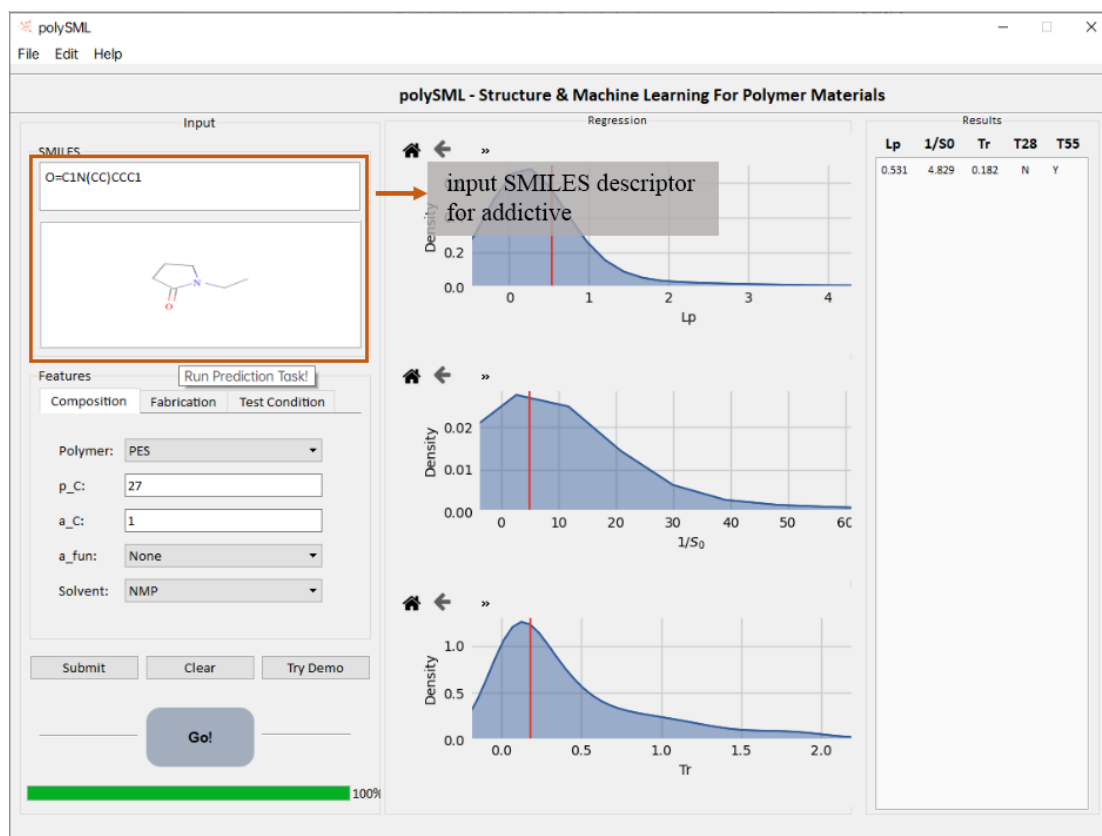
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Win7/vista/win8/win10, 105M RAM, 400M storage

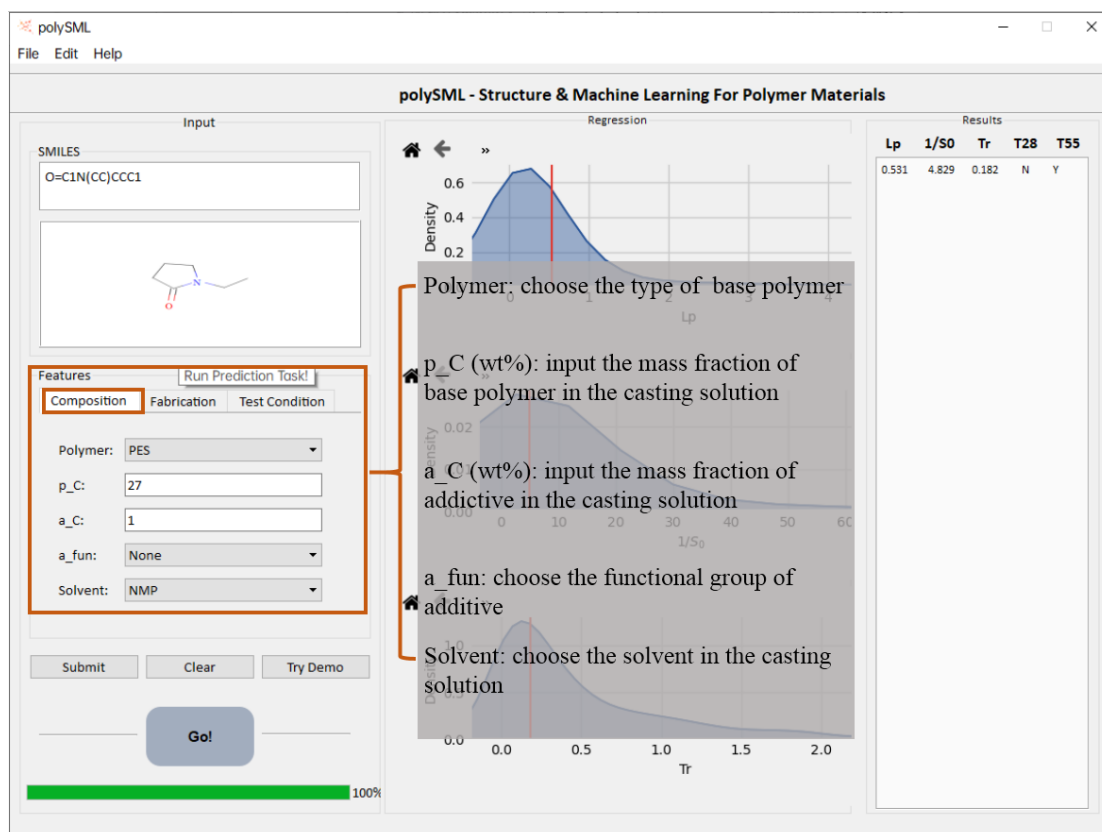
## 2 Usage

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1. Input correct **SMILES** for additive in polymer solution (SMILES can be queried from Pubchem <https://pubchem.ncbi.nlm.nih.gov/> ).



## 2. Parameters for composition, fabrication and test condition.



polySML

File Edit Help

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Input

SMILES

O=C1N(CC)CCC1

Features

Composition **Fabrication** Test Condition

nonsolvent: Water

coag\_T: 20

wet\_mem\_thick: 100

exposed\_time: 0

pre\_T: 20

Submit Clear Try Demo

Go!

100%

Regression

Density

0.6

0.4

0.2

0.0

0.0 0.5 1.0 1.5 2.0

Tr

Results

Lp	1/S0	Tr	T28	T55
0.531	4.829	0.182	N	Y

nonsolvent: choose the nonsolvent in the coagulation bath

coag\_T (°C): input the temperature of coagulation bath

wet\_mem\_thick (μm): input the thickness of wet membrane

exposed\_time (s): solvent evaporation time before immersion into coagulation bath

pre\_T (°C): the temperature of casting solution

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File Edit Help

polySML - Structure & Machine Learning For Polymer Materials

Input

SMILES

O=C1N(CC)CCC1

Features

Composition Fabrication **Test Condition**

rej\_type: Salt

rej\_r: HSA

rej\_charge: -1

rej\_C: 2

flux\_P: 200

Submit Clear Try Demo

Go!

100%

Regression

Density

0.6

0.4

0.2

0.0

0.0 0.5 1.0 1.5 2.0

Tr

Results

Lp	1/S0	Tr	T28	T55
0.531	4.829	0.182	N	Y

rej\_type: choose the type of substance to be filtered

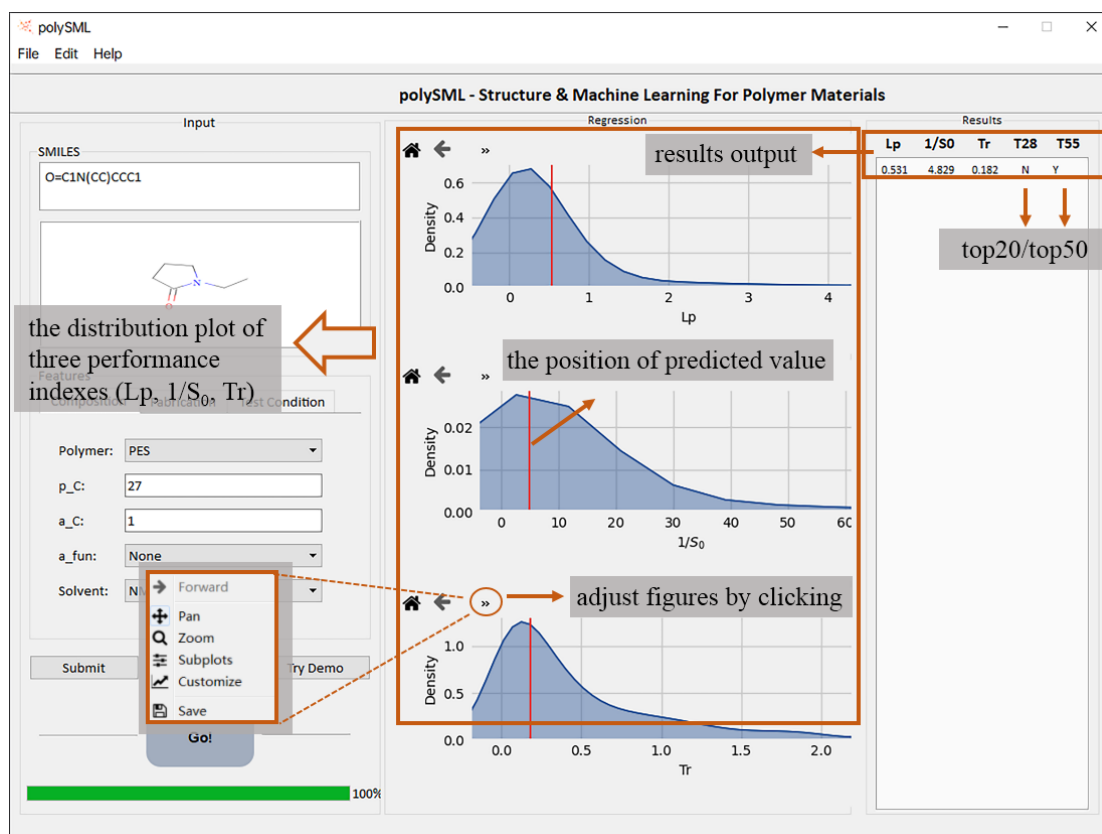
rej\_r (nm): choose the substance to be filtered

rej\_charge (C): input the charge of ion if the substance to be filtered is salt

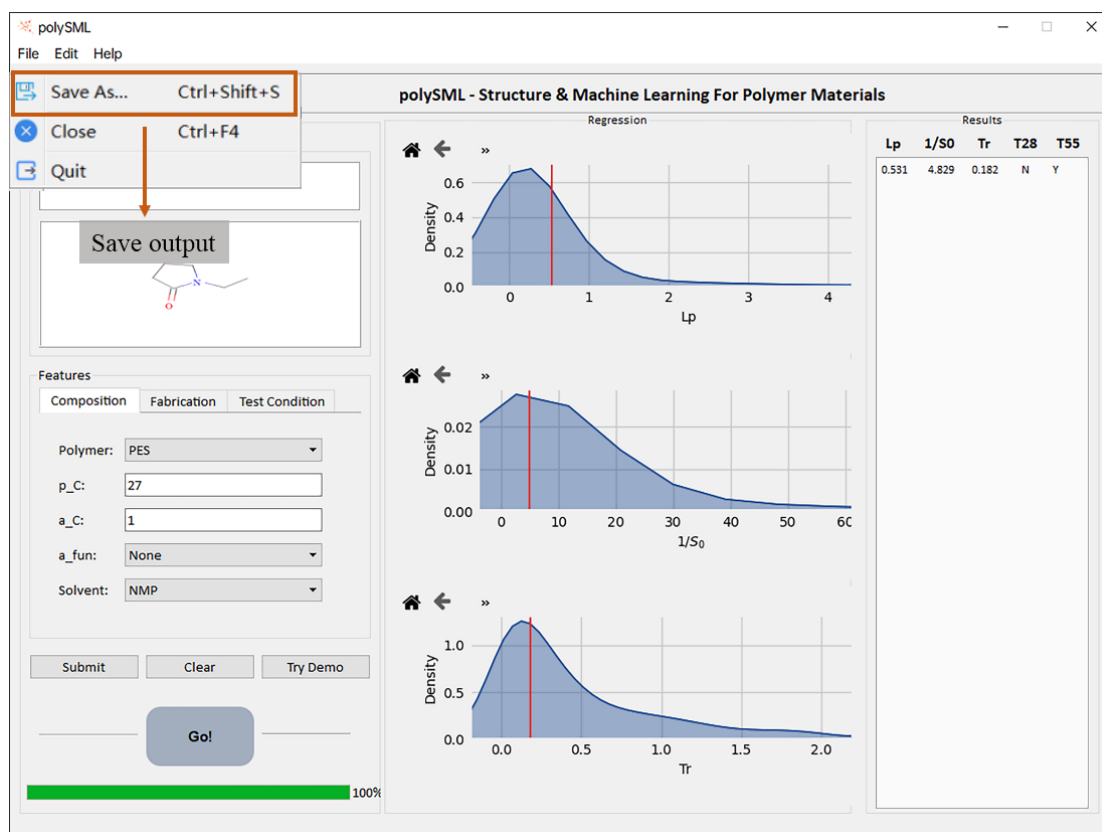
rej\_C (g/l): input the concentration of substance

flux\_P (kPa): the transmembrane pressure applied to the membrane

3. Click **Submit** and check all the inputs correct.
4. Click **GO** for predictions.



5. Click **Save As** to save outputs.



## 3 Predictor: WFM\_poly

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This model provides the prediction for three critical performance indexes accounting micro-/ultra-/nano-filtration membranes and the evaluation of the overall membrane performance grade.

### 3.1 Regression models

#### Permeability( $L_p$ )

The permeability is defined as:

$$L_p = \frac{J_v}{\Delta P \times p_0} \quad (1)$$

Where  $J_v$  is the volumetric filtrate flux (m/s),  $\Delta P$  is the transmembrane pressure (Pa),  $p_0$  is the unit permeability coefficient ( $10^{-9} \text{ m} \cdot \text{s}^{-1} \text{ Pa}^{-1}$ )

#### Selectivity( $1/S_0$ )

The selectivity is defined as:

$$1/S_0 = (1 - R)^{-1} = \frac{C_f}{C_p} \quad (2)$$

Where  $R$  is the rejection ratio (%),  $C_p$  and  $C_f$  are the concentrations of substances in the permeation and feed flux (wt%).

#### Trade-off coefficient( $T_r$ )

The trade-off coefficient of defined as:

$$T_r = \frac{2 \times L_p \times 1/s_0}{L_p + 1/s_0} \quad (3)$$

### 3.2 Classification models

According to the "trade-off curve", we got four curves which can divide the macromolecules and salts data points into 50:50 and 20:80. The output result

is "Y" means that the performance of the membrane is above the trade-off curve, on the contrary, the result is "N".

## Features

Features used for prediction models are listed below:

ID	Feature	Unit	Description
1	p_C	wt%	The weight fraction of base polymer in casting solution
2	a_C	wt%	The weight fraction of the additive in casting solution
3	s_C	wt%	The weight fraction of the solvent in casting solution
4	s_Dis	-	Hansen solubility parameter (Dispersion force for solvent)
5	p_Dis	-	Hansen solubility parameter (Dispersion force for monomer in polymer)
6	RED_S	-	The relative energy difference between base polymer and solvent
7	RED_NS	-	The relative energy difference between base polymer and non-solvent
8	Bp	°C	Boiling point for solvent and non-solvent
9	Vp	mmHg	The saturated vapor pressure at 25°C for solvent and non-solvent
10	HDT	°C	Heat Deflection Temperature with loading of 1.8MPa
11	coag_T	°C	The temperature of coagulation bath
12	pre_T	°C	The temperature during membrane formation
13	exposed.time	s	The exposed time before immersing the casting solution into the non-solvent
14	wet_mem_thick	μm	The thickness of solution on the substrate controlled by the scraper
15	flux_P	kPa	Transmembrane pressure in performance measurement
16	rej_C	wt%	The concentration of substance (protein, salt etc.) in feeding flux
17	rej_type	-	The type of separation substance
18	rej_charge	C	The charge of separation substance
19	rej_r	nm	The radius of rejection substance
20	porosity	%	Volume fraction of water accessible voids in membrane
21	CA	°	Water static contact angle on membrane surface

## 4 License

The copyright for this software suite is owe to the authors, academic free for current version and commercial usages please contact the corresponding author [yunqi@ciac.ac.cn](mailto:yunqi@ciac.ac.cn).

## 5 References

Users are encouraged to cite the following references for special predictors.

1. Liu T, Liu L, Cui F, Ding F, & Li Y Predict the performance of Polyvinylidene fluoride, polyethersulfone and polysulfone micro/ultra/nano-filtration membranes, 2020, submitted.
2. Liu L, Chen W, Liu T, Kong X, Zheng J, & Li Y Rational design of hydrocarbon-based sulfonated copolymers for proton exchange membranes J. Mater. Chem. A, 2019 7:11847-11857.
3. Liu L, Chen W, & Li Y A Statistical Study of Proton Conduction in Nafion<sup>®</sup>-based Composite Membranes: Prediction, Filler Selection and Fabrication Methods J. Membr. Sci., 2018 549:393-402.
4. Liu L, Chen W, & Li Y An overview of the proton conductivity of nafion membranes through a statistical analysis J. Membr. Sci., 2016 504:1-9.

**Release log:** 201912 version v0.0.1, construct the UI and common block. WFM\_poly model was integrated. 202003 version v1 predictor about polymer materials for water filtration membranes(WFM\_poly) was integrated.

## 6 Limitation

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Current models mainly focus on the types of polymers, additions, solvents reported. For novel compounds, chemical structures, predictions are made based on knowledge, confidence needs validation in blind-test. We are not guarantee the prediction is fully accurate but guidelines are possible.

## 7 Bug report and suggestions

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Please contact either [lyliu@ciac.ac.cn](mailto:lyliu@ciac.ac.cn) or [yunqi@ciac.ac.cn](mailto:yunqi@ciac.ac.cn) for bugs or suggestions.

## 8 About us

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We are a research group dedicating in structure and machine learning study on polymer materials. We are welcoming suggestions and collaborations. Contact Prof. Yunqi Li for further information.