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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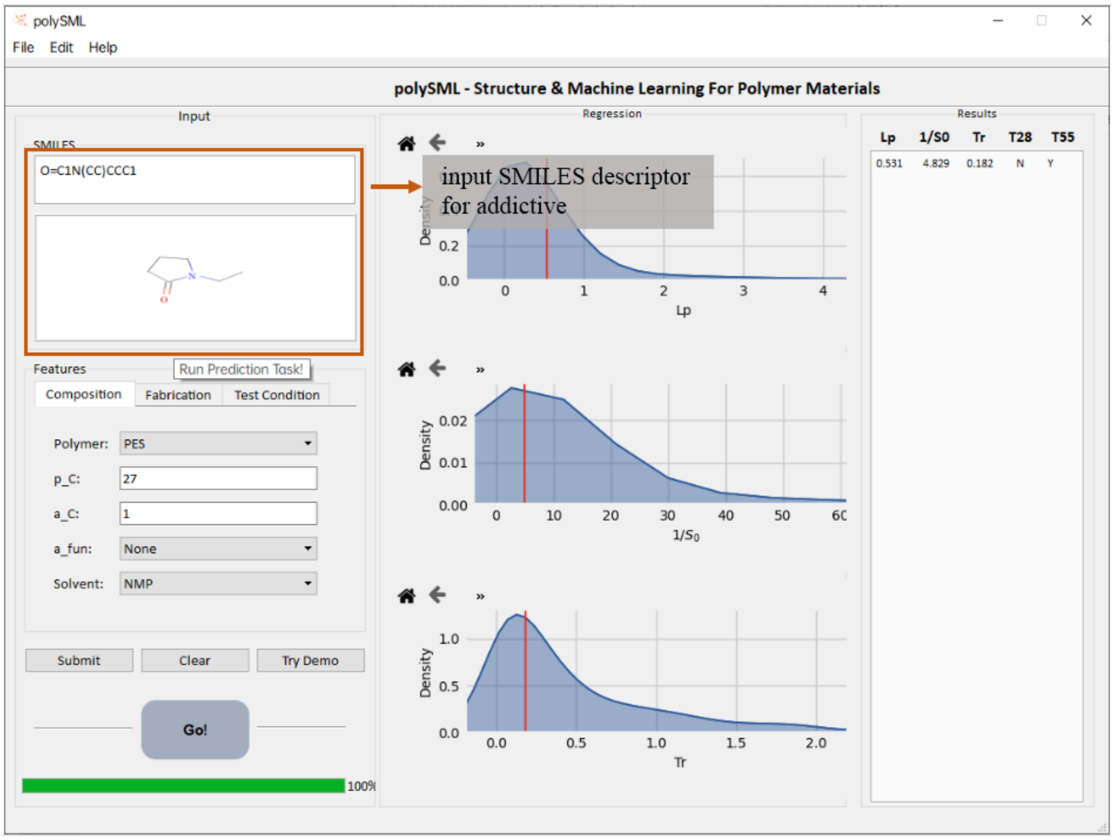
1 Requirements

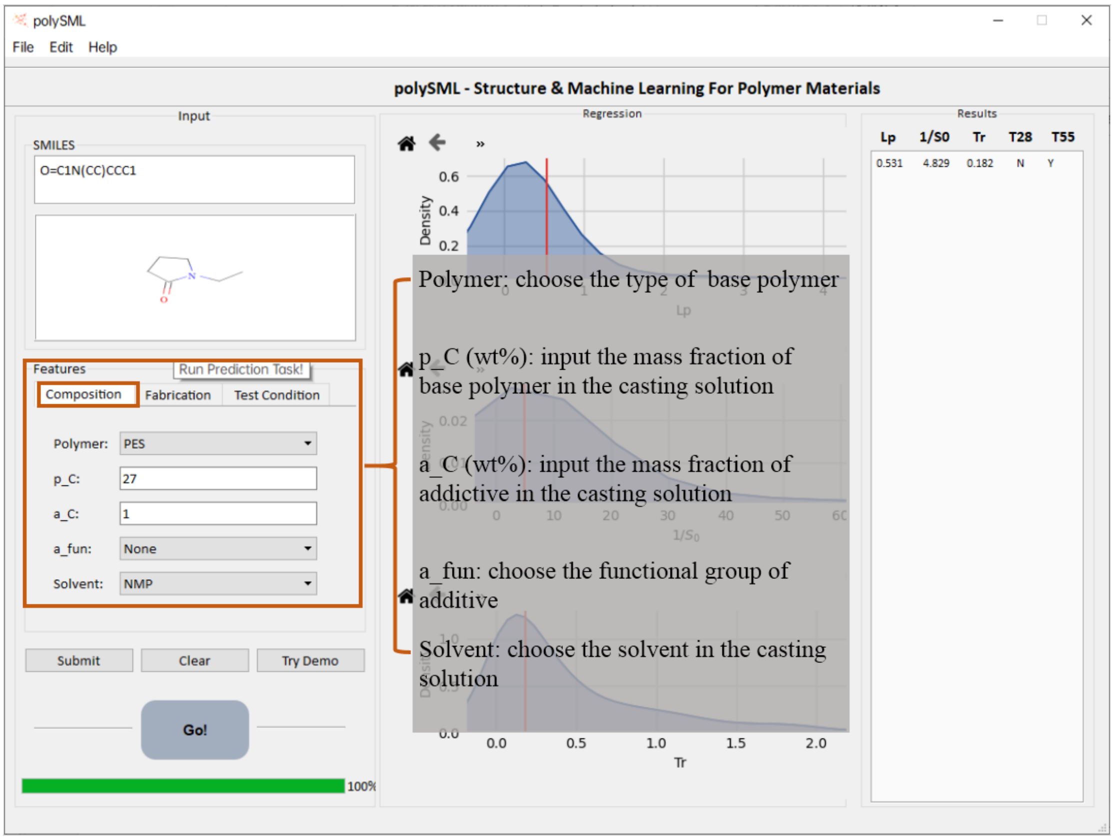
Win7/vista/win8/win10, 105M RAM, 400M storage

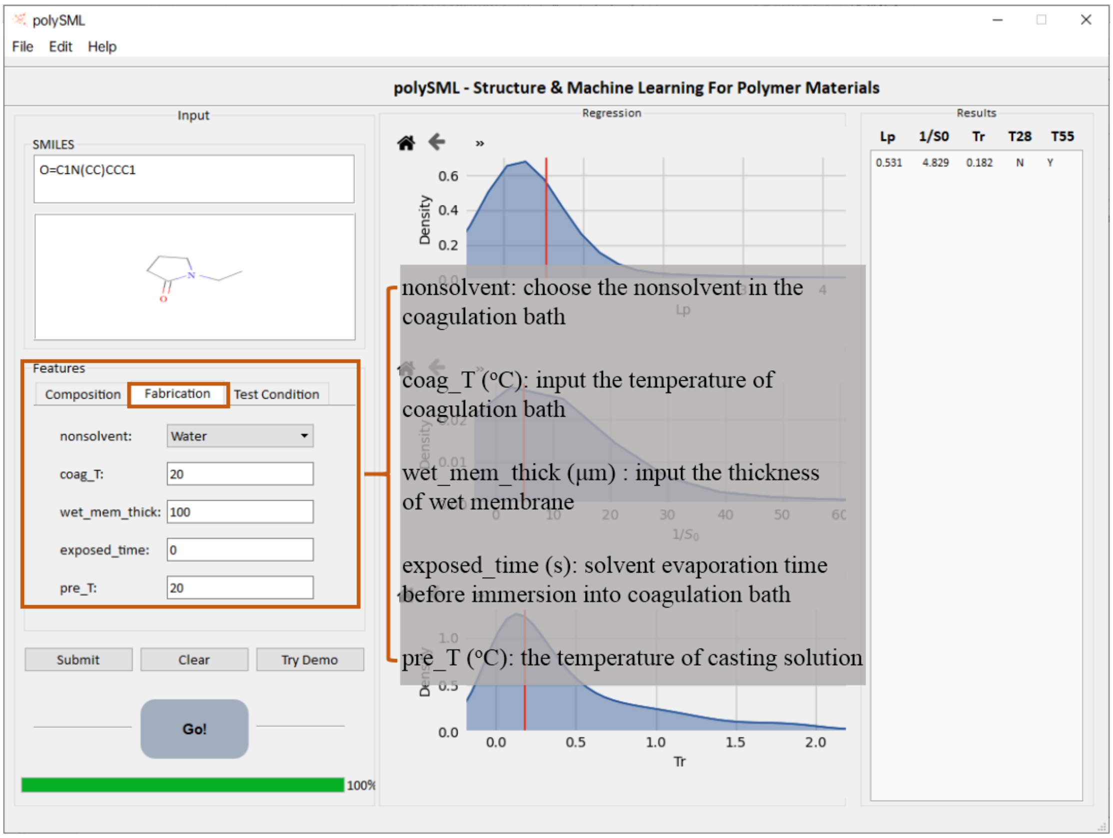
2 Usage

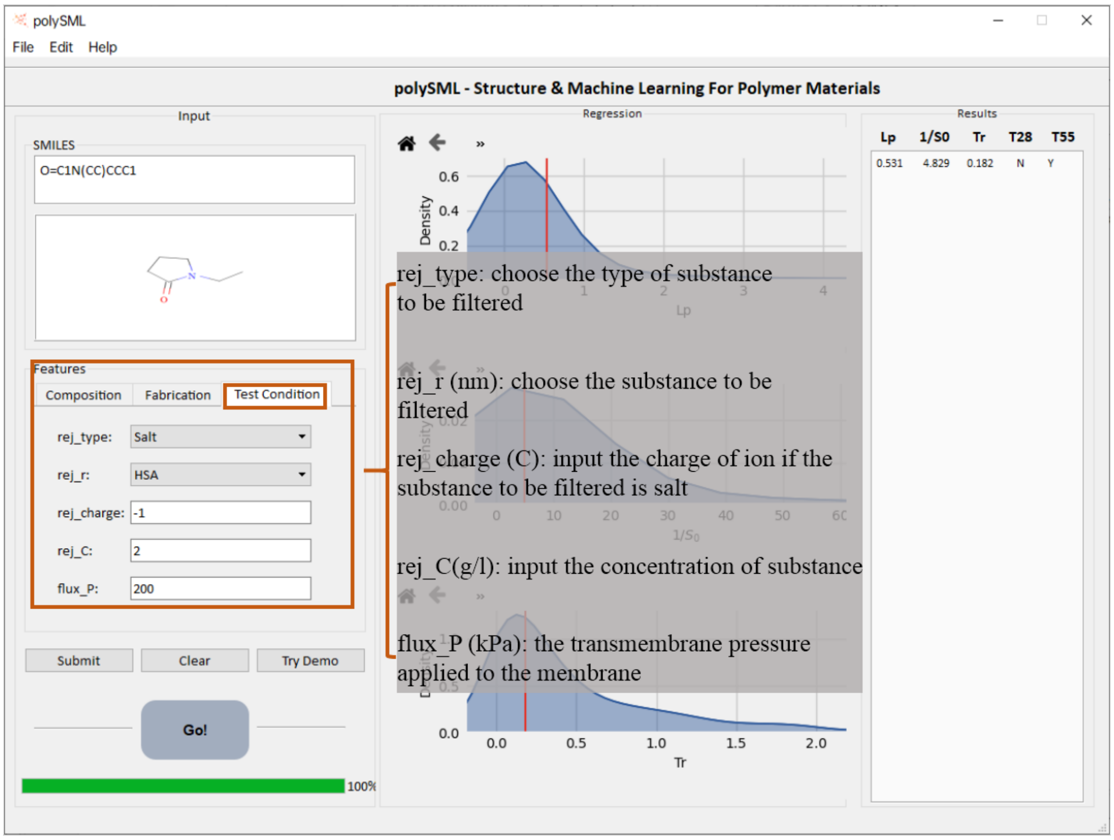
1. Input correct **SMILES** for addictive in polymer solution (SMILES can be queried from Pubchem https://pubchem.ncbi.nlm.nih.gov/).



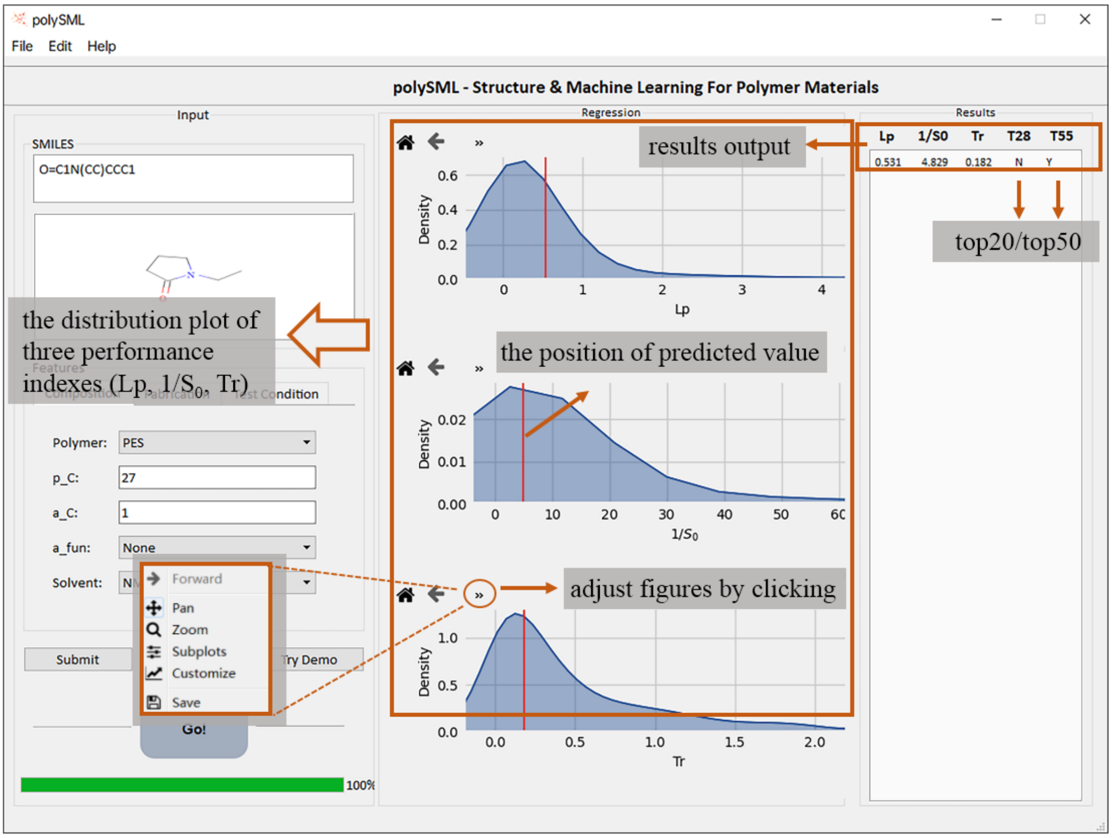
2. Parameters for **composition, fabrication** and **test condition**.



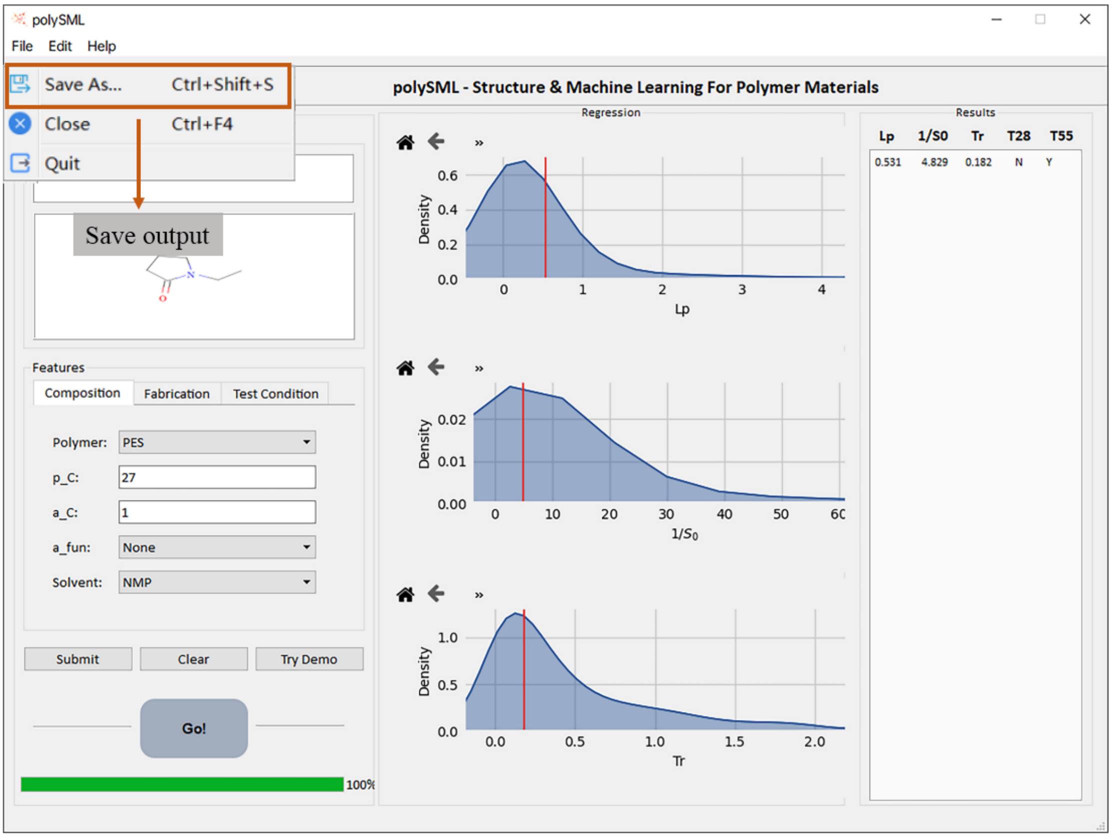




3. Click **Submit** and check all the inputs correct.
4. Click **GO** for predictions.



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



3 Predictor: WFM_poly

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(Lp)

The permeability is defined as:

$$Lp = \frac{J_v}{\Delta P \times p_0} \tag{1}$$

Where J_v is the volumetric filtrate flux (m/s), ΔP is the transmembrane pressure (Pa), p_0 is the unit permeability coefficient (10^{-9} m·s^{-1} Pa^{-1})

Selectivity(1/S_0)

The selectivity is defined as:

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

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(Tr)

The trade-off coefficient of defined as:

$$T_r = \frac{2 \times Lp \times 1/s_0}{\mathrm{Lp} + 1/s_0} \tag{3}$$

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 addictive in casting solution
3	s_C	wt%	The weight fraction of the solvent in casting solution
4	s_Disp	-	Hansen solubility parameter (Dispersion force for solvent)
5	p_Disp	-	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	ºC	Boiling point for solvent and non-solvent
9	Vp	mmHg	The saturated vapor pressure at 25ºC for solvent and non-solvent
10	HDT	ºC	Heat Deflection Temperature with loading of 1.8MPa
11	coag_T	ºC	The temperature of coagulation bath
12	pre_T	ºC	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	º	Water static contact angle on membrane surface

4 License

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, ployethersulfone 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?-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

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

Please contact either lyliu@ciac.ac.cn or yunqi@ciac.ac.cn for bugs or suggestions.

8 About us

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.