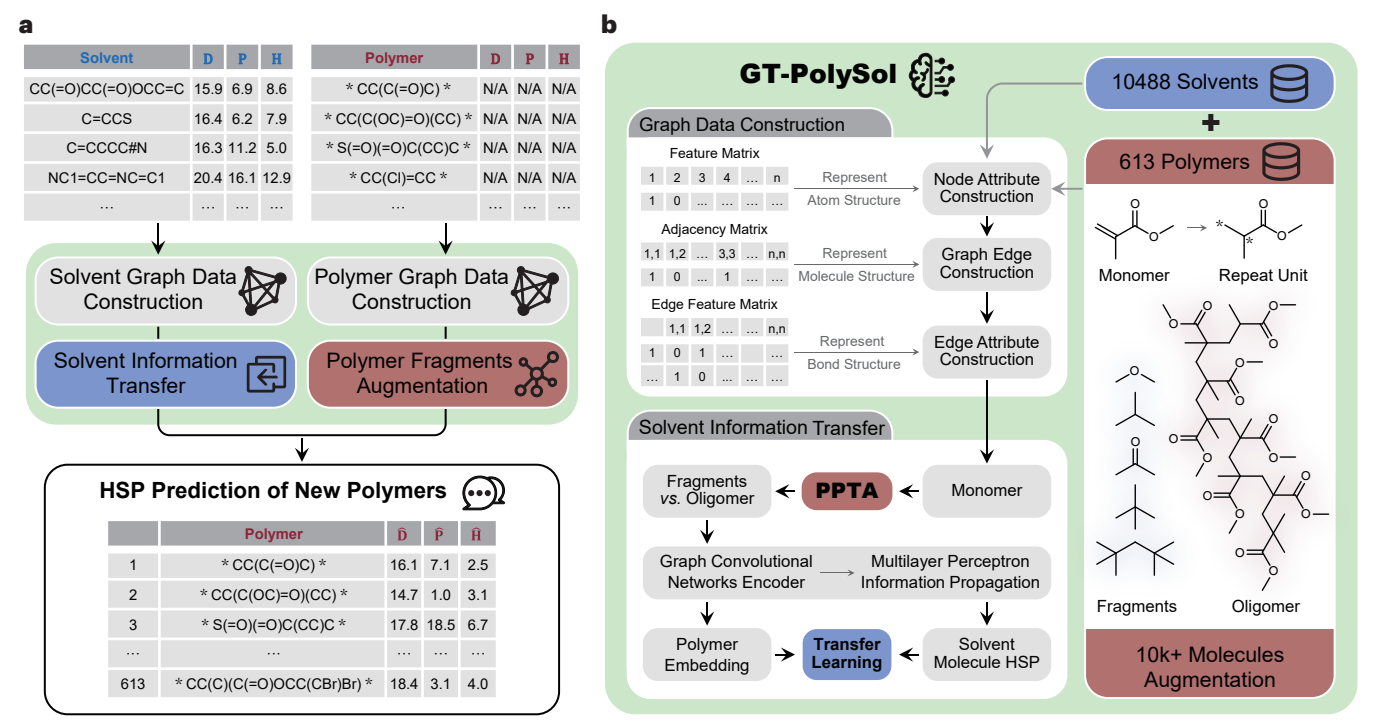
a
Solvent
D
P
H
CC(=O)CC(=O)OCC=C
15.9
6.9
8.6
C=CCS
16.4
6.2
7.9
C=CCCC#N
16.3
11.2
5.0
NC1=CC=NC=C1
20.4
16.1
12.9
Polymer
* CC(C(=O)C) *
N/A
* CC(C(OC)=O)(CC) *
* S(=O)(=O)C(CC)C *
* CC(Cl)=CC *
Solvent Graph Data Construction
Polymer Graph Data Construction
Solvent Information Transfer
Polymer Fragments Augmentation
HSP Prediction of New Polymers
Polymer
1
* CC(C(=O)C) *
16.1
7.1
2.5
2
* CC(C(OC)=O)(CC) *
14.7
1.0
3.1
3
* S(=O)(=O)C(CC)C *
17.8
18.5
6.7
613
* CC(C)(C(=O)OCC(CBr)Br) *
18.4
3.1
4.0
b
GT-PolySol
10488 Solvents
613 Polymers
Graph Data Construction
Feature Matrix
Represent
Atom Structure
Node Attribute Construction
Adjacency Matrix
Represent
Molecule Structure
Graph Edge Construction
Edge Feature Matrix
Represent
Bond Structure
Edge Attribute Construction
Monomer
Repeat Unit
Fragments
Oligomer
Solvent Information Transfer
Fragments vs. Oligomer
PPTA
Monomer
Graph Convolutional Networks Encoder
Multilayer Perceptron Information Propagation
Polymer Embedding
Transfer Learning
Solvent Molecule HSP
10k+ Molecules Augmentation