COSMOlogic培训

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输运性质 – 液相热导 (LTC)

纯物质 + QSPR + 单位 (W/m/s)

$$\kappa_i = c_0 + c_{Visc}\eta_i + c_{MW}MW_i + c_{Tr2}T_{r,i}^2 \quad T_r = T/T_c$$

其中:

c_0，c_{Visc}，c_{MW}，c_{Tr2} 分别为参数，由COSMOlogic软件的参数文件 (.ctd)提供

T_c 为临界温度 (critical temperature)

MW_i 为摩尔质量 $\quad\quad \eta_i$ 为纯物质粘度

LTC_param={c_0 c_{Visc} c_{MW} c_{Tr2}} 可自行定义上述四个参数

粘度和临界温度，COSMOtherm可自行预测，也可以通过编辑vap文件读取，或在命令行给出实验值，后两种方法的优先级高于COSMOtherm自行预测。

输运性质 – 扩散系数（DC）

无限稀释模型下扩散系数 + 纯或混合溶剂 + QSPR + 单位(m^2/s)

$$D_i = c_0 + c_{lnT} \ln(T)$$
$$+ c_{muH}^{Solute}\left(\mu_i^{S,\infty} - H_i^{S,\infty}\right) + c_{Area}^{Solute} A_i + c_{M2}^{Solute} M_i^{(2)}$$
$$+ c_{H_{tot}}^{Solvent} H_S + c_{H_{MF}}^{Solvent}\left(E_S^{diel} + H_S^{MF}\right) + c_{H_{HB}}^{Solvent} H_S^{HB} + c_{H_{vdW}}^{Solvent} H_S^{vdW} + c_{N_{Ring}}^{Solvent} N_S^{Ring}$$

diffcoeff[=i]：指定溶剂编号；

Ndiffcoeff=namei：指定溶剂名称。

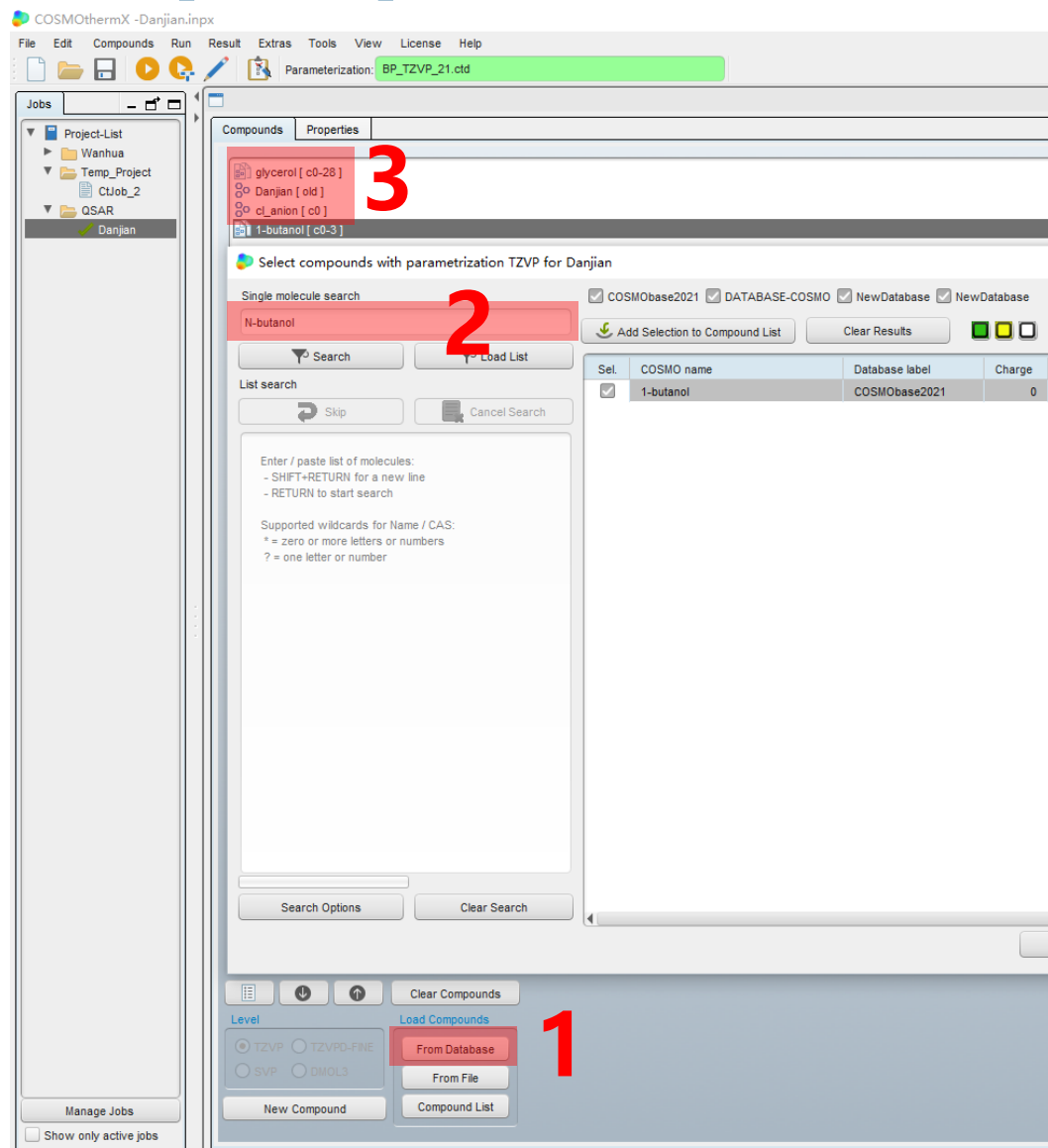上述两个参数不指定，给出混合比例（摩尔比x={...}或质量比c={...}），则采用混合溶剂。

输运性质 – 扩散系数（DC）

扩散系数计算是由命令行方式实现！

为了简化工作：

1，基于COSMOthermX图形界面的活度系数预测功能，如下图：

输运性质 – 扩散系数（DC）

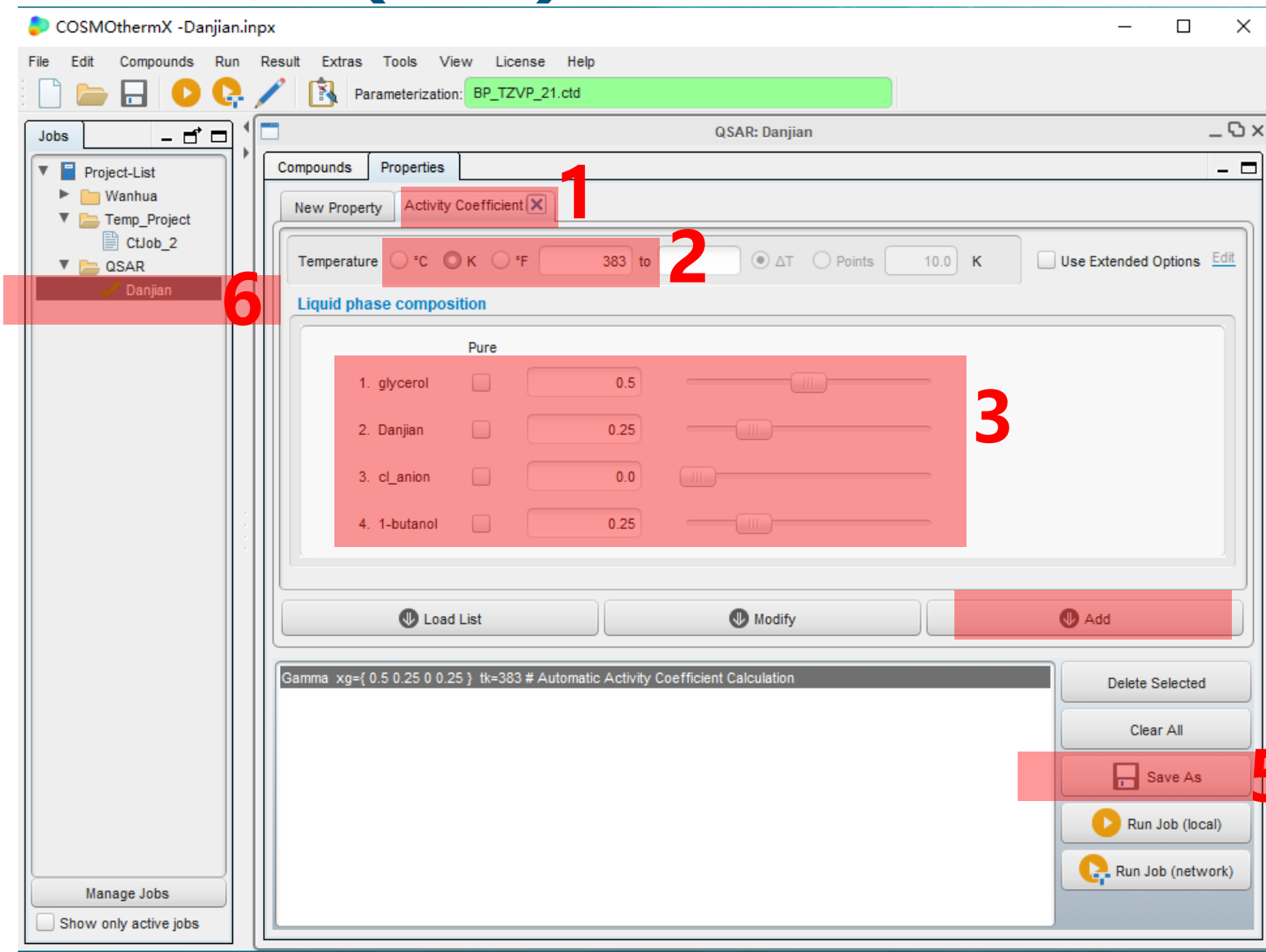## 2，选择"Properties"中的"Activity Coefficient"。
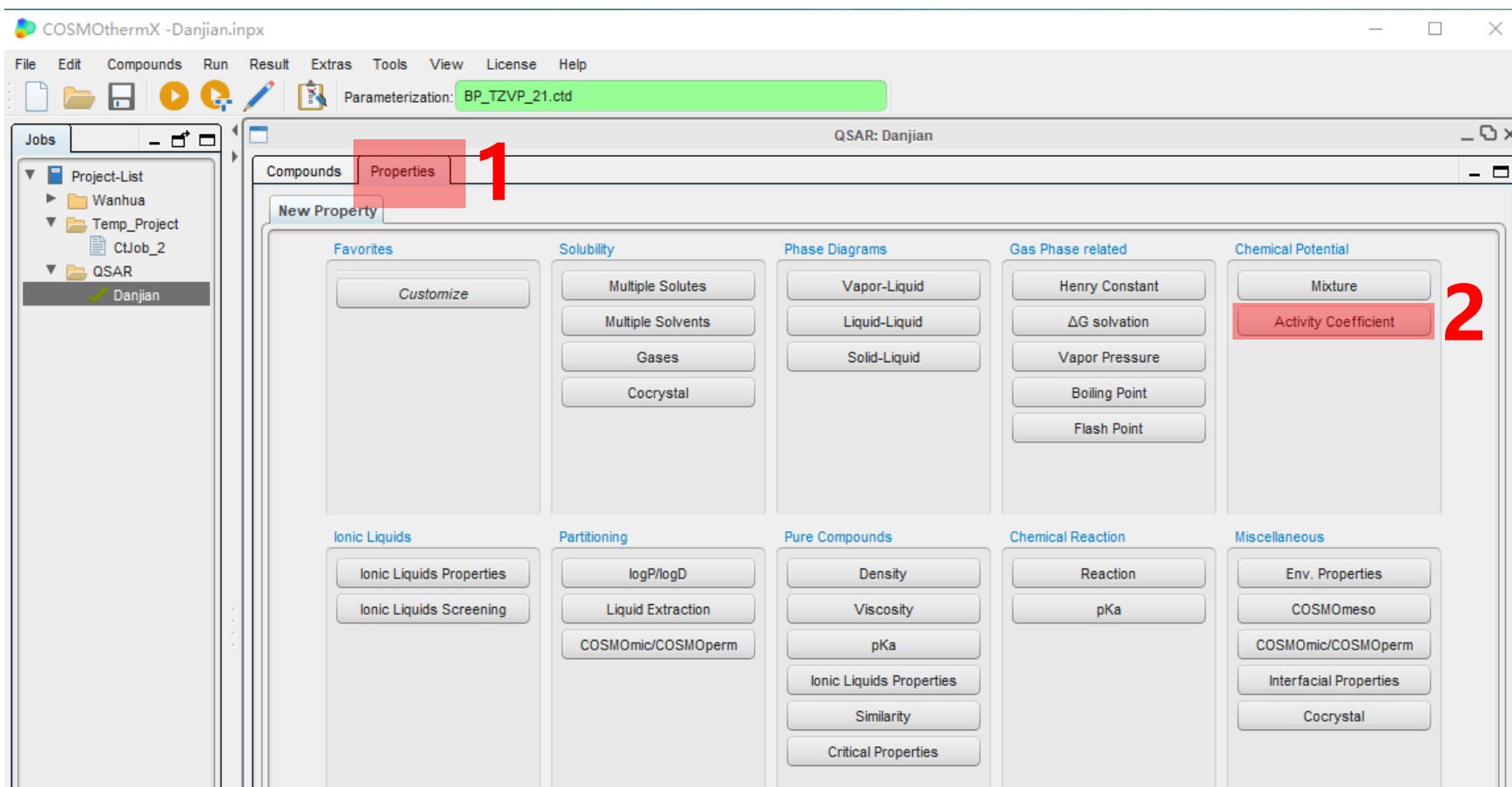
输运性质 – 扩散系数（DC）

3，设置
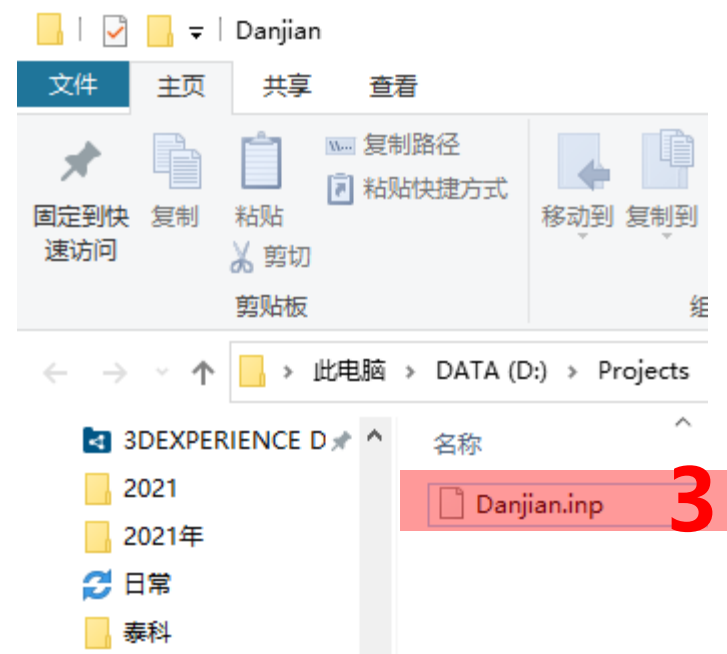
"Temperature" 383

K，选择溶剂各组分的

摩尔比，点击"Add"，

点击"Save As"，命

名为，如"Danjian"。

输运性质 – 扩散系数（DC）

4，鼠标右键点击任务 "Danjian"，选择 "View Job Directory"。
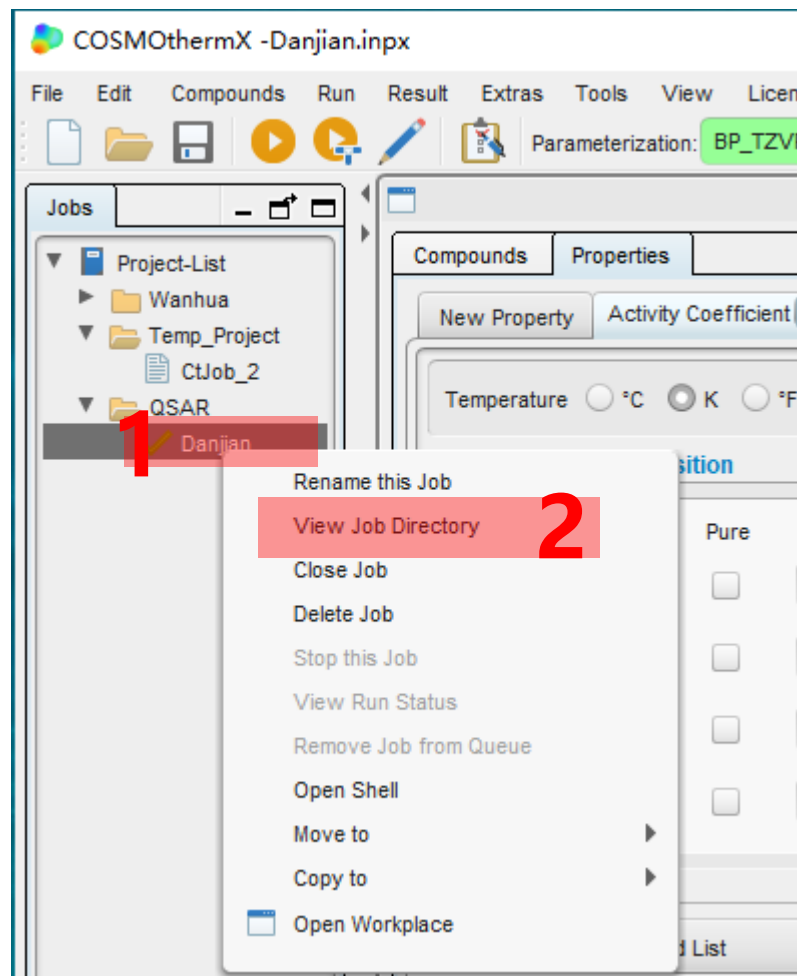
输运性质 – 扩散系数（DC）

5，用文本编辑器编辑"Danjian.inp"文件，修改最后一行为，如2。

```
 1  ctd = BP_TZVP_21.ctd cdir = "C:\Program Files\BIOVIA\COSMOtherm2021\COSMOthermX\..\COSMOtherm\CTDATA-FILES" ldir = "C:\Program Files\BIOVIA\COSMOtherm2021\COSMOthermX\..\lic
 2  notempty wtln ehfile
 3  !! generated by COSMOthermX !!
 4  f = "glycerol_c0.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"    Comp = "glycerol" [  VPfile
 5  f = "glycerol_c1.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
 6  f = "glycerol_c2.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
 7  f = "glycerol_c3.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
 8  f = "glycerol_c4.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
 9  f = "glycerol_c5.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
10  f = "glycerol_c6.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
11  f = "glycerol_c7.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
12  f = "glycerol_c8.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
13  f = "glycerol_c9.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
14  f = "glycerol_c10.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
15  f = "glycerol_c11.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
16  f = "glycerol_c12.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
17  f = "glycerol_c13.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
18  f = "glycerol_c14.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
19  f = "glycerol_c15.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
20  f = "glycerol_c16.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
21  f = "glycerol_c17.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
22  f = "glycerol_c18.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
23  f = "glycerol_c19.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
24  f = "glycerol_c20.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
25  f = "glycerol_c21.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
26  f = "glycerol_c22.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
27  f = "glycerol_c23.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
28  f = "glycerol_c24.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
29  f = "glycerol_c25.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
30  f = "glycerol_c26.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
31  f = "glycerol_c27.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\g"
```

2 **Diffcoeff x={ 0.5 0.25 0 0.25 } tk=383**

```
35  f = "1-butanol_c0.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\1"    Comp = "1-butanol" [  VPfile
36  f = "1-butanol_c1.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\1"
37  f = "1-butanol_c2.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\1"
38  f = "1-butanol_c3.cosmo" fdir="D:\Chemsofts\BIOVIA\2021\BIOVIA_2021.AM_COSMObase_2021\COSMObase2021\BP-TZVP-COSMO\1"    ]
39  Gamma  xg={ 0.5 0.25 0 0.25 }  tk=383 # Automatic Activity Coefficient Calculation
```

1

输运性质－扩散系数（DC）

6，保存退出编辑，再鼠标右键点击"Danjian"，

"Open Shell"，

输入"cosmotherm Danjian.inp"，运行。

输运性质 – 扩散系数（DC）

7，鼠标右键点击 "Danjian"，"View Job Directory"
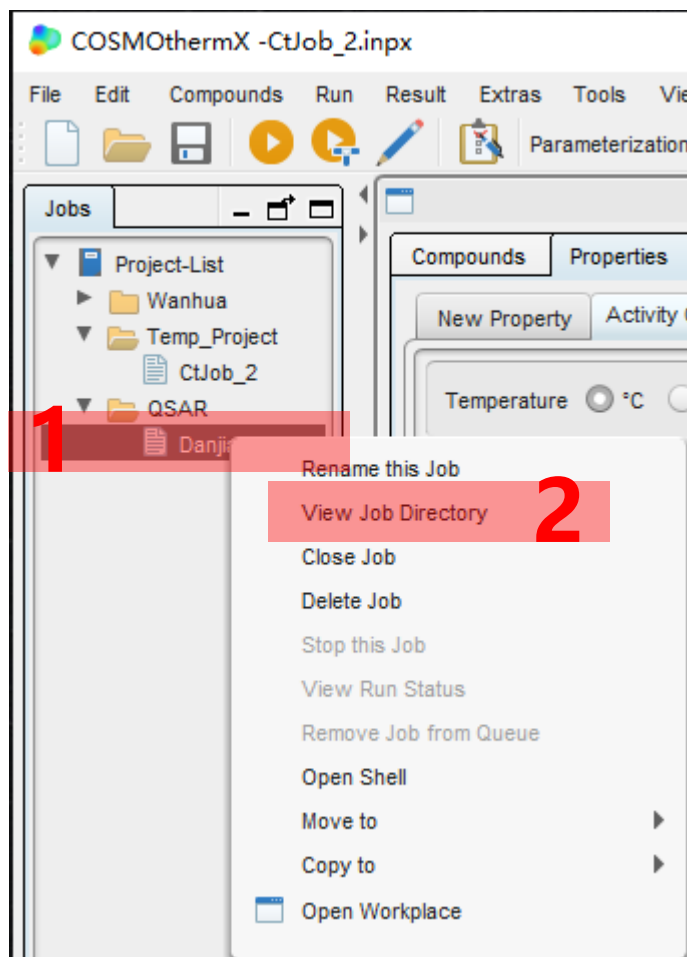
输运性质 – 扩散系数 (DC)

7，文本编辑器打开"Danjian.tab"，结果是1，2是单位。

```
Property   job 1 : Infinite Dilution Diffusion Coefficient ;
Settings   job 1 : T= 298.15 K ; x(1)= 0.2500 x(3)= 0.5000 x(4)= 0.2500 ;
Units      job 1 : Diffusion Coefficient in m^2/s  2

Nr Compound                              DIFFC
 1 Danjian                              1.2758E-10
 2 1-butanol                            1.4321E-10  1
 3 glycerol                             1.4029E-10
 4 cl_anion                             1.9445E-10
```

温度与扩散系数

```
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=-5.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=5.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=15.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=25.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=35.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=45.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=55.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=65.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=75.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=85.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=95.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=105.0 # Automatic Activity Coefficient Calculation
diffcoeff x={ 0.25 0 0.5 0.25 }    tc=110.0 # Automatic Activity Coefficient Calculation
```
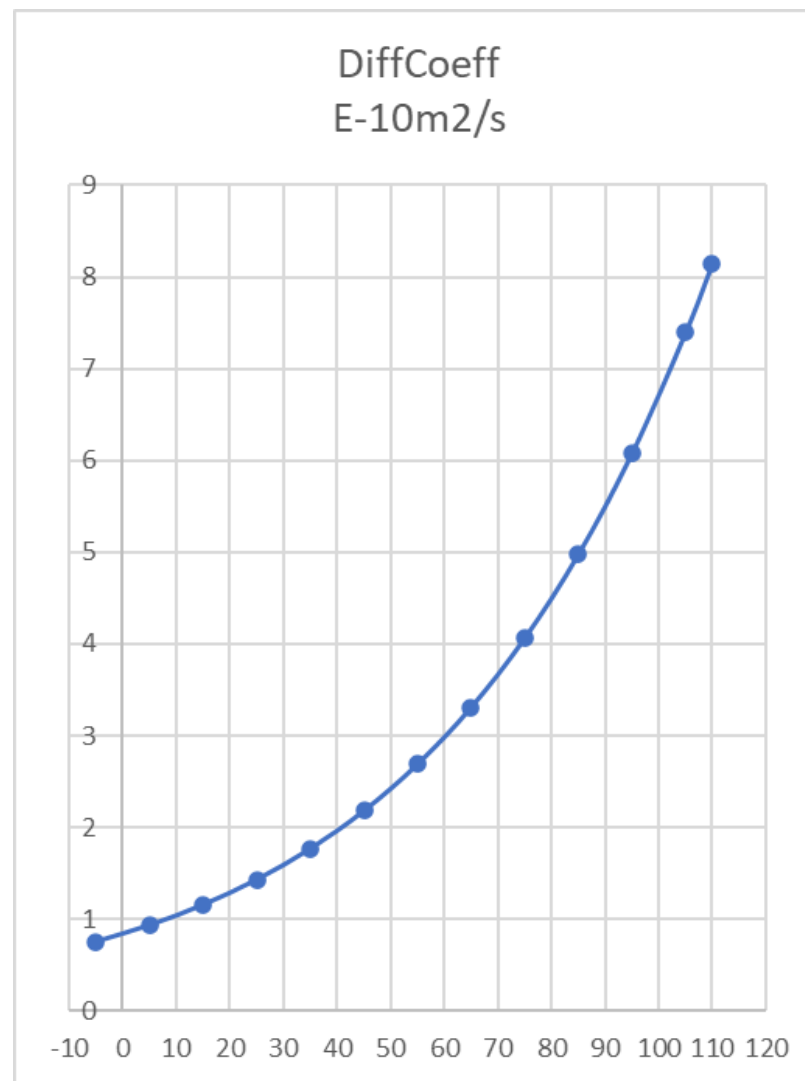
温度与扩散系数

温度 摄氏度	扩散系数 E-10m2/s
-5	0.7535
5	0.9348
15	1.1578
25	1.4321
35	1.7694
45	2.1836
55	2.6912
65	3.3112
75	4.0657
85	4.9792
95	6.0792
105	7.3953
110	8.1441

扩散系数 E-10m2/s
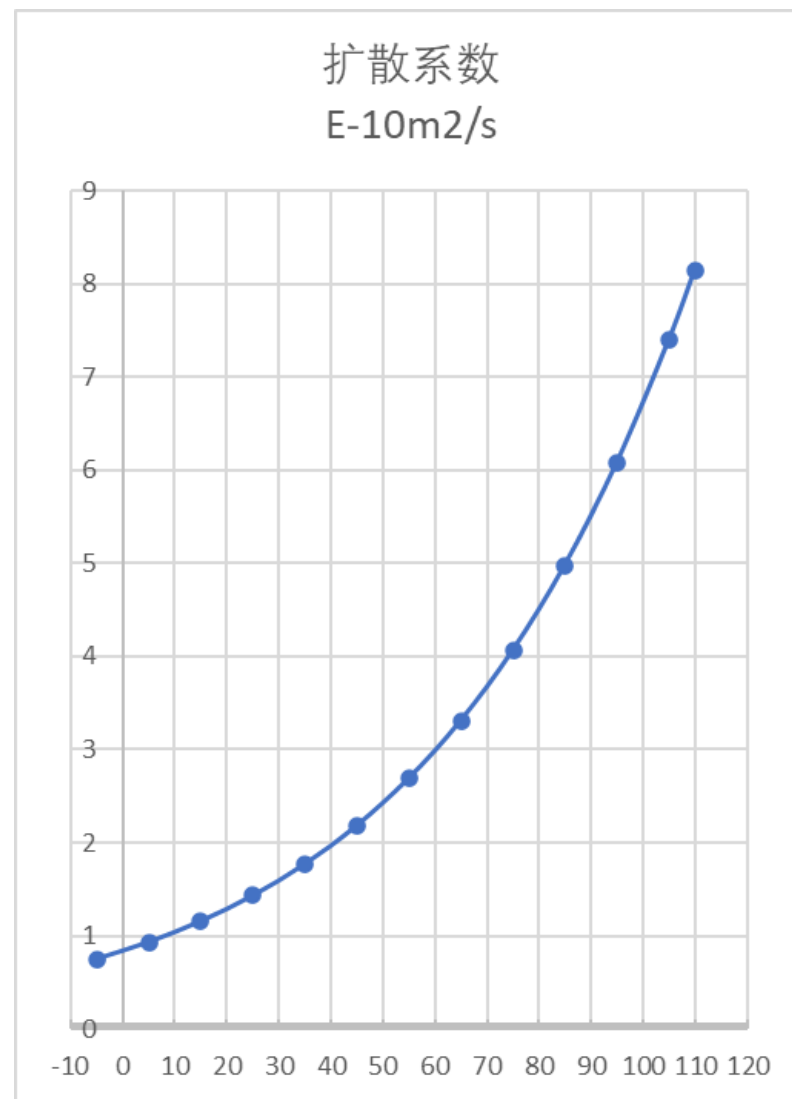
T and Diffusion Coefficient

T (Celsius)	DiffCoeff E-10m2/s
-5	0.7535
5	0.9348
15	1.1578
25	1.4321
35	1.7694
45	2.1836
55	2.6912
65	3.3112
75	4.0657
85	4.9792
95	6.0792
105	7.3953
110	8.1441

DiffCoeff E-10m2/s

机器学习方法

基于COSMOtherm的sigma-profile描述符的线性或多线性回归模型（QSPR）很难正确描述固体的热力学性质。

基于机器学习（ML）方法，结合拓扑结构和自由能描述符，可以很好的描述上述性质，特别是Tmelt、Hfusion性质。

目前版本的COSMOtherm提供随机森林（Random Forest）算法或梯度提升（Gradient Boosting Model）算法

机器学习方法

命令行方式实现！

为了简化工作：

1，基于COSMOthermX图
形界面的活度系数预测功能，
导入化合物。

如右图：
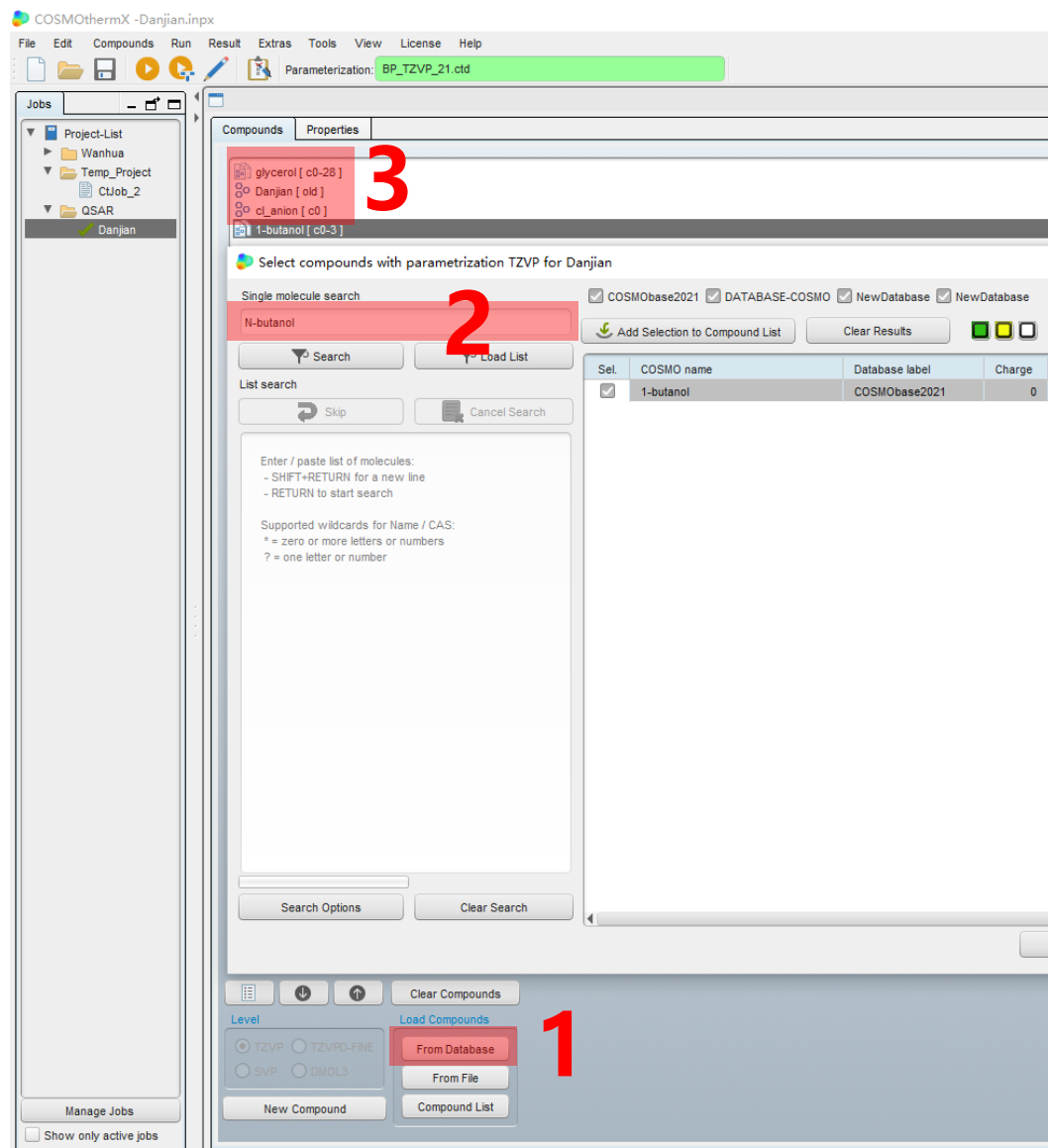
机器学习方法

2，选择"Properties"中的"Activity Coefficient"。
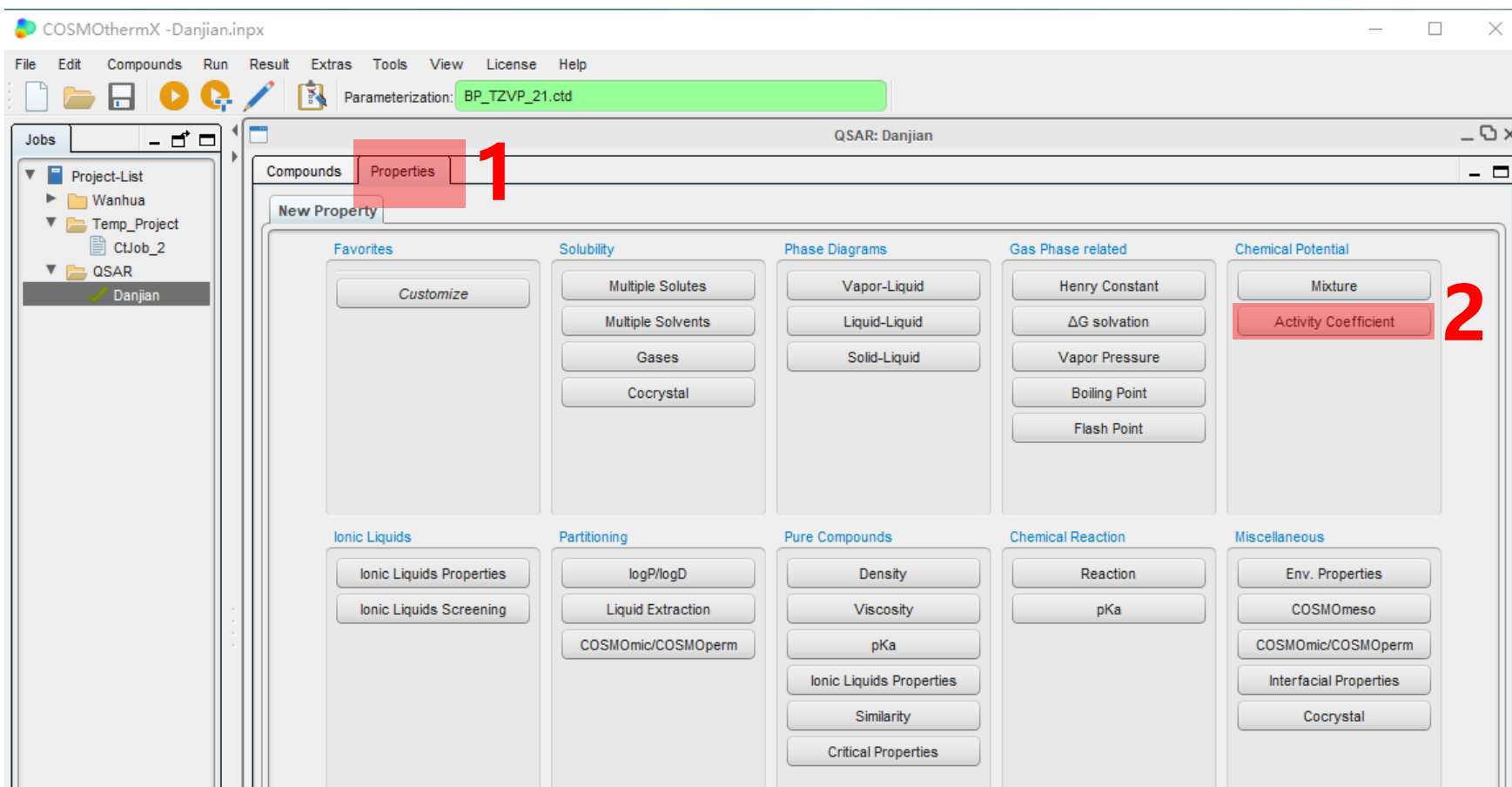
机器学习方法

3，设置温度、液相组分等参数。
注意，这些参数对熔融焓和熔点计算没有影响。

4，点击"Save As"。
如，
存成"rfmodel"。

机器学习方法

5，鼠标右键点击任务"rfmodel"，选择"View Job Directory"。

6，用文本编辑器打开"rfmodel.inp"。
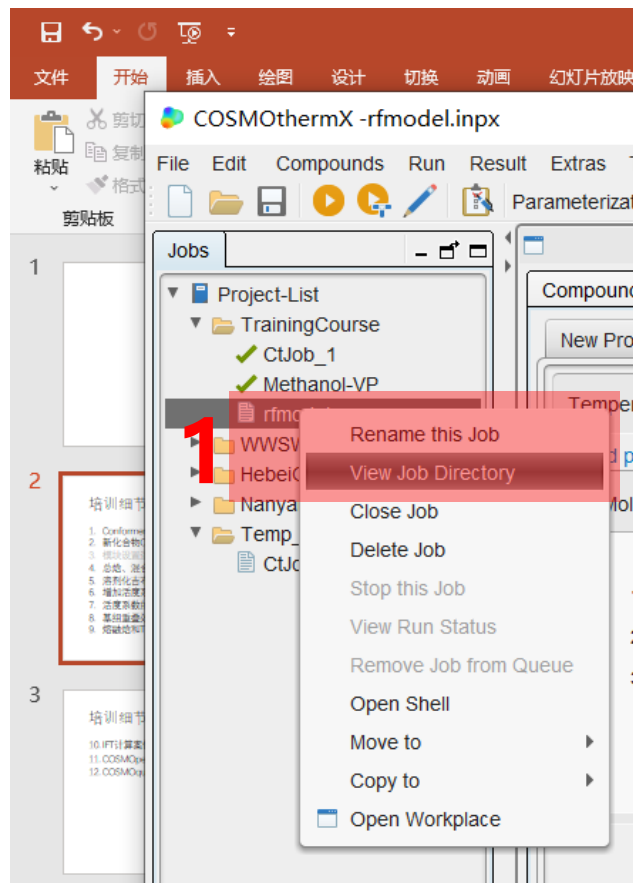
机器学习方法

7，删除原来计算活度系数的命令行，增加熔融焓和熔点的命令，如右图：

8，存盘推出。


```
ctd = BP_TZVP_22.ctd cdir = "C:\Program Files\BIOV:
notempty wtln ehfile
!! generated by COSMOthermX !!
f = "h2o_c0.cosmo" fdir="C:\Program Files\BIOVIA\C(
f = "1-octanol_c0.cosmo" fdir="C:\Program Files\BI(
f = "1-octanol_c1.cosmo" fdir="C:\Program Files\BI(
f = "1-octanol_c2.cosmo" fdir="C:\Program Files\BI(
f = "1-octanol_c3.cosmo" fdir="C:\Program Files\BI(
f = "1-octanol_c4.cosmo" fdir="C:\Program Files\BI(
f = "1-octanol_c5.cosmo" fdir="C:\Program Files\BI(
f = "1-octanol_c6.cosmo" fdir="C:\Program Files\BI(
f = "4-aminonitrobenzene_c0.cosmo" fdir="C:\Progra1
```

1 `##Gamma=1 tc=25.0 # Automatic Activity Coefficient`

2
```
RFMODEL=MeltingPoint_FINE.propx tc=25 x_pure=1
RFMODEL=Hfusion_FINE.propx tc=25 x_pure=1
```
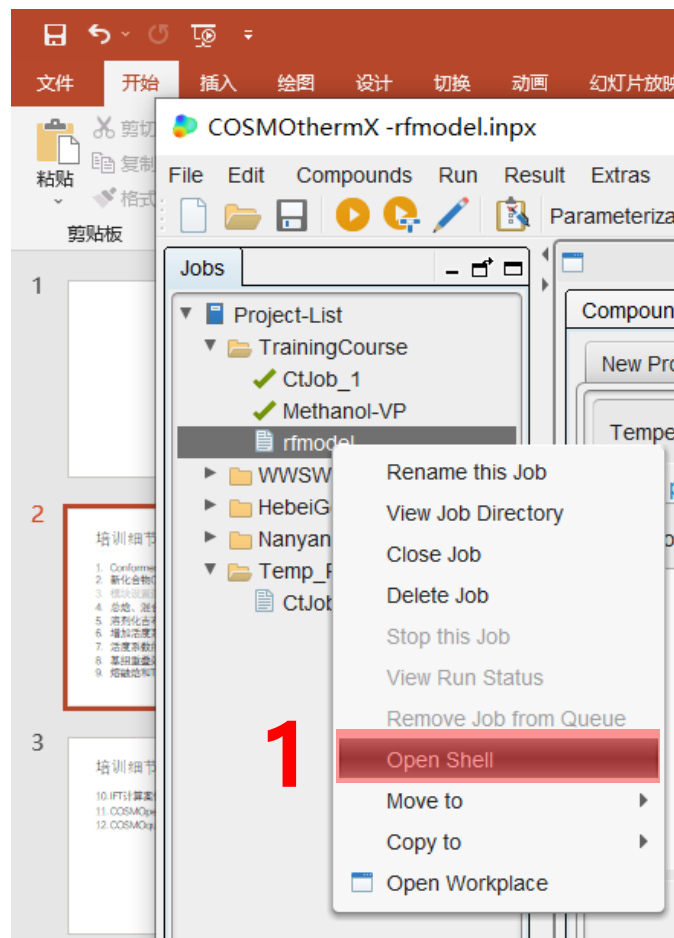
机器学习方法

9，鼠标右键点击任务 "rfmodel"，选择 "Open Shell"。

10，执行命令：

cosmoterm rfmodel.inpu

机器学习方法

11，鼠标右键点击任务 "rfmodel"，选择 "View Job Directory"。

12，用文本编辑器打开 "rfmodel.tab"。

13，按构象和化合物分别给出熔融焓和熔点。
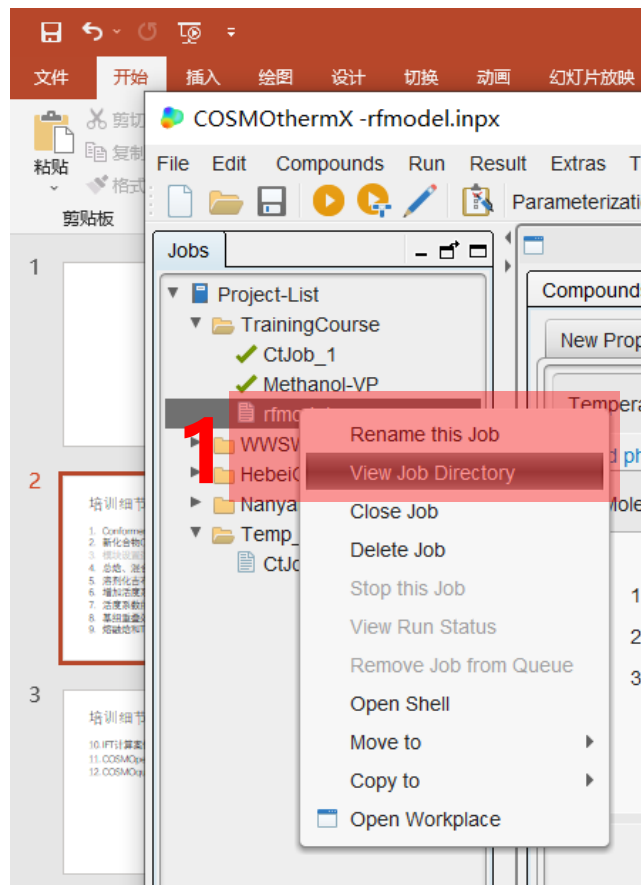
机器学习方法

注意：

RFMODEL=MeltingPoint_**FINE**.propx tc=25 x_pure=1
RFMODEL=Hfusion_**FINE**.propx tc=25 x_pure=1

上述命令中红色标出的部分，要与导入的化合物level一致。对应关系如下：

SVP = SVP

TZVP = TZVP

TZVPD-Fine = FINE

DMOL3 = DMOL3