How to use the tool?


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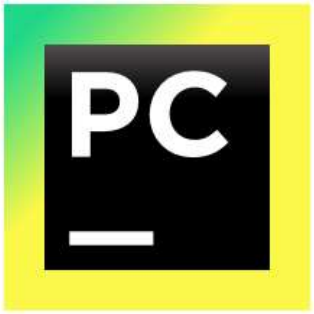
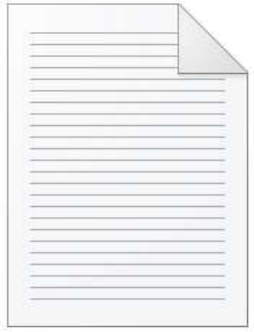
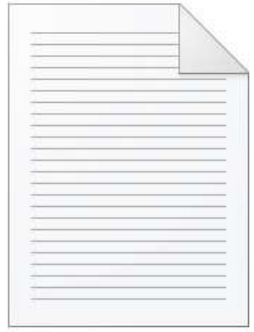

DecIDE.py


Input.xlsx


Output.xlsx


ReadMe.txt


requirements.txt

Read me file: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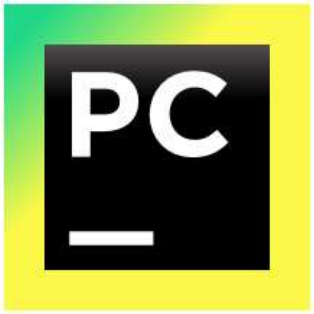
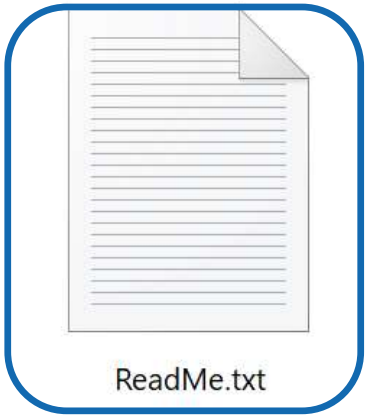
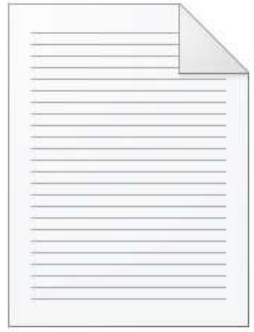

DecIDE.py


Input.xlsx


Output.xlsx


ReadMe.txt


requirements.txt

Package version overview: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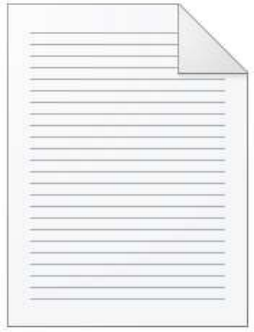
Input.xlsx


Output.xlsx


ReadMe.txt


requirements.txt

Optional: Copy your DIPPR Database files here: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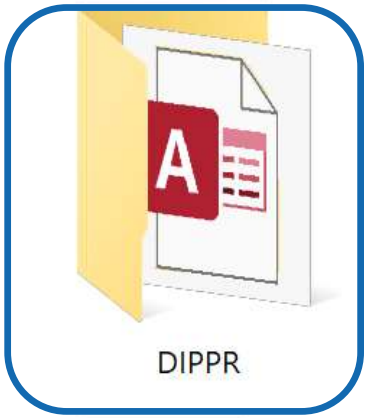
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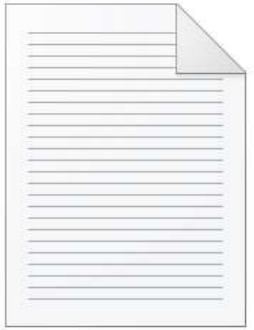
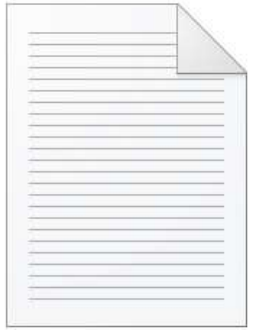
DecIDE.py


Input.xlsx


Output.xlsx


ReadMe.txt


requirements.txt

Enter the reaction equations here: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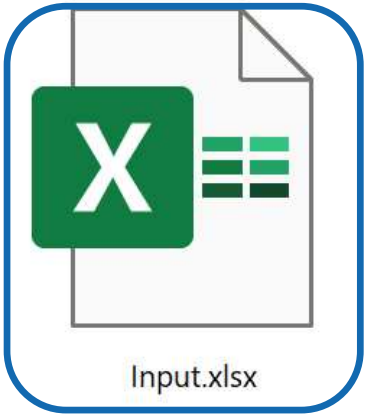
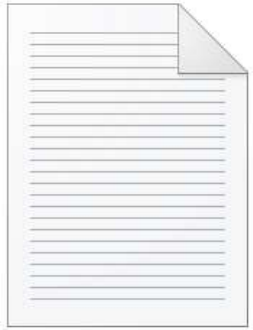
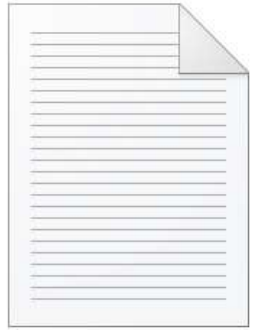

Input.xlsx


Output.xlsx


ReadMe.txt


requirements.txt

Input for automatic generation of features:
- Add CAS Numbers

	A	B	C	D	E	F	G	H	I	J	K
1	**Feature name:**	**Number**	**Name**	**Mainproduct (CAS)**	**Product 1 (CAS)**	**Product 2 (CAS)**	**Mainproduct (stoich)**	**Product 1 (stoich)**	**Product 2 (stoich)**	**Reactant 1 (CAS)**	**Reactant 2 (CAS)**
2	*Short description of the feature:*	*Your own identifier for your reaction/process*	*Your own name for this reaction/process*	*CAS-No of Mainproduct, Format: …XX-XX-X (https://commonchemistry.cas.org/)*	*CAS-No of Product 1, Format: …XX-XX-X*	*CAS-No of Product 2, Format: …XX-XX-X*	*Stoichiometric coefficient of Mainproduct*	*Stoichiometric coefficient of Product 1*	*Stoichiometric coefficient of Product 2*	*CAS-No of Reactant 1, Format: …XX-XX-X*	*CAS-No of Reactant 2, Format: …XX-XX-X*
3	*Your reactions:*	1	1,3-Butadiene	106-99-0	7732-18-5	1333-74-0	1	2	1	64-17-5	
4		2	Acetaldehyde	75-07-0	7732-18-5		2	2		64-17-5	7782-44-7
5											

Input for automatic generation of features:
- Add CAS Numbers

	A	B	C	D	E	F	G	H	I	J	K
1	**Feature name:**	**Number**	**Name**	**Mainproduct (CAS)**	**Product 1 (CAS)**	**Product 2 (CAS)**	**Mainproduct (stoich)**	**Product 1 (stoich)**	**Product 2 (stoich)**	**Reactant 1 (CAS)**	**Reactant 2 (CAS)**
2	*Short description of the feature:*	*Your own identifier for your reaction/process*	*Your own name for this reaction/process*	*CAS-No of Mainproduct, Format: …XX-XX-X (https://commonchemistry.cas.org/)*	*CAS-No of Product 1, Format: …XX-XX-X*	*CAS-No of Product 2, Format: …XX-XX-X*	*Stoichiometric coefficient of Mainproduct*	*Stoichiometric coefficient of Product 1*	*Stoichiometric coefficient of Product 2*	*CAS-No of Reactant 1, Format: …XX-XX-X*	*CAS-No of Reactant 2, Format: …XX-XX-X*
3	*Your reactions:*	1	1,3-Butadiene	106-99-0	7732-18-5	1333-74-0	1	2	1	64-17-5	
4		2	Acetaldehyde	75-07-0	7732-18-5		2	2		64-17-5	7782-44-7
5											

Input for automatic generation of features:
- Add CAS Numbers
- Add stoichiometric coefficients

	A	B	C	D	E	F	G	H	I	J	K
1	**Feature name:**	**Number**	**Name**	**Mainproduct (CAS)**	**Product 1 (CAS)**	**Product 2 (CAS)**	**Mainproduct (stoich)**	**Product 1 (stoich)**	**Product 2 (stoich)**	**Reactant 1 (CAS)**	**Reactant 2 (CAS)**
2	*Short description of the feature:*	*Your own identifier for your reaction/process*	*Your own name for this reaction/process*	*CAS-No of Mainproduct, Format: …XX-XX-X (https://commonchemistry.cas.org/)*	*CAS-No of Product 1, Format: …XX-XX-X*	*CAS-No of Product 2, Format: …XX-XX-X*	*Stoichiometric coefficient of Mainproduct*	*Stoichiometric coefficient of Product 1*	*Stoichiometric coefficient of Product 2*	*CAS-No of Reactant 1, Format: …XX-XX-X*	*CAS-No of Reactant 2, Format: …XX-XX-X*
3	*Your reactions:*	1	1,3-Butadiene	106-99-0	7732-18-5	1333-74-0	1	2	1	64-17-5	
4		2	Acetaldehyde	75-07-0	7732-18-5		2	2		64-17-5	7782-44-7
5											

Input for automatic generation of features :
- Add CAS Numbers
- Add stoichiometric coefficients
- Same for reactants
- Add Number and Name and copy Number and Name to the first sheet

	A	B	C	D	E	F	G	H	I	J	K
1	**Feature name:**	**Number**	**Name**	**Mainproduct (CAS)**	**Product 1 (CAS)**	**Product 2 (CAS)**	**Mainproduct (stoich)**	**Product 1 (stoich)**	**Product 2 (stoich)**	**Reactant 1 (CAS)**	**Reactant 2 (CAS)**
2	*Short description of the feature:*	*Your own identifier for your reaction/process*	*Your own name for this reaction/process*	*CAS-No of Mainproduct, Format: ...XX-XX-X (https://commonchemistry.cas.org/)*	*CAS-No of Product 1, Format: ...XX-XX-X*	*CAS-No of Product 2, Format: ...XX-XX-X*	*Stoichiometric coefficient of Mainproduct*	*Stoichiometric coefficient of Product 1*	*Stoichiometric coefficient of Product 2*	*CAS-No of Reactant 1, Format: ...XX-XX-X*	*CAS-No of Reactant 2, Format: ...XX-XX-X*
3	*Your reactions:*	1	1,3-Butadiene	106-99-0	7732-18-5	1333-74-0	1	2	1	64-17-5	
4		2	Acetaldehyde	75-07-0	7732-18-5		2	2		64-17-5	7782-44-7
5											

Run the code to generate required features and outputs: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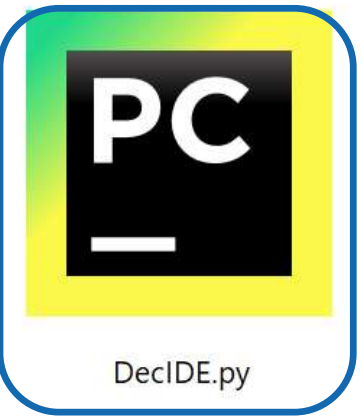
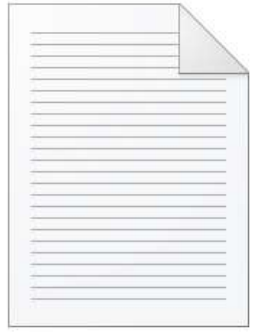

DecIDE.py

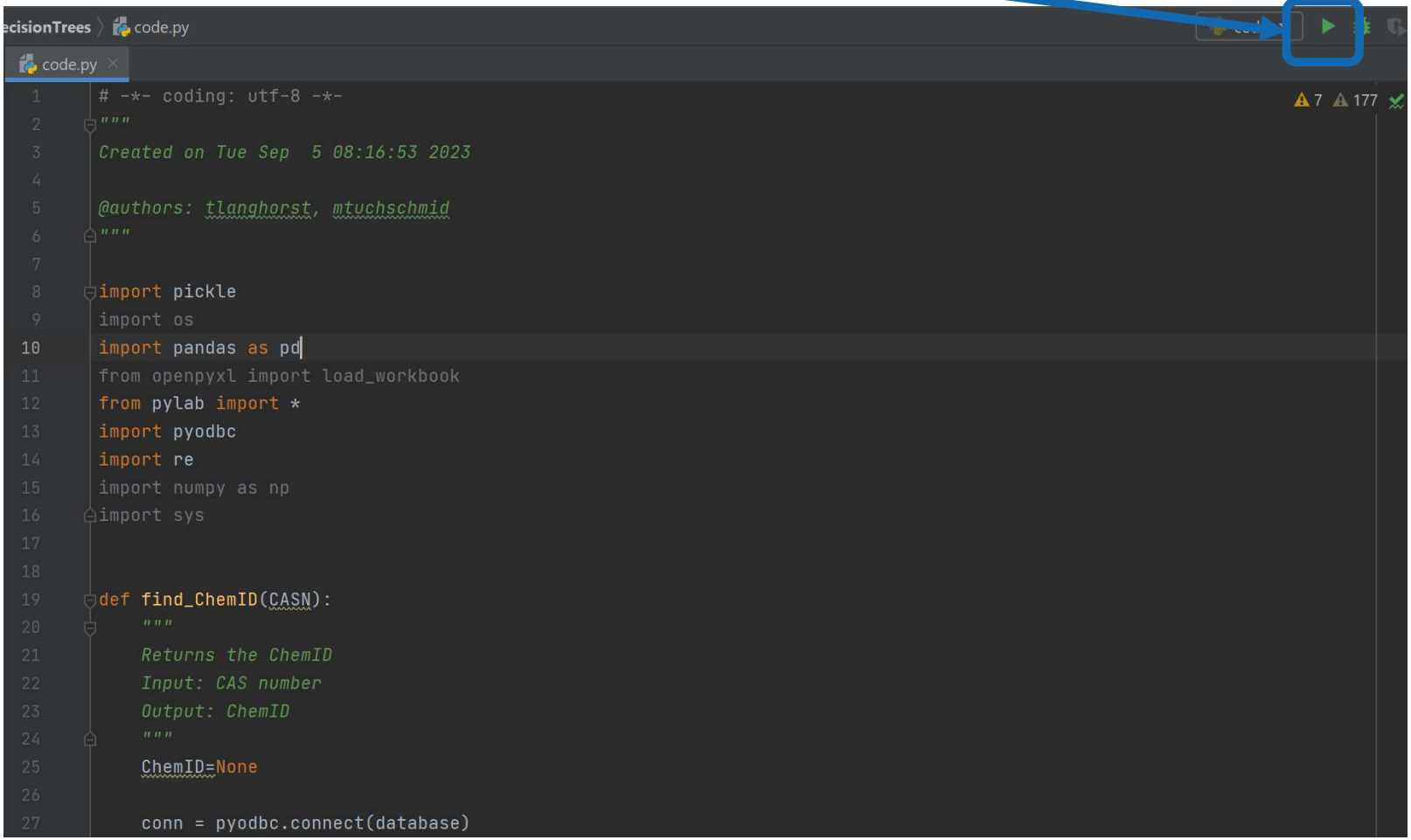

Input.xlsx


Output.xlsx


ReadMe.txt


requirements.txt

All you need to do is click on run



Manual input of features or check automated input: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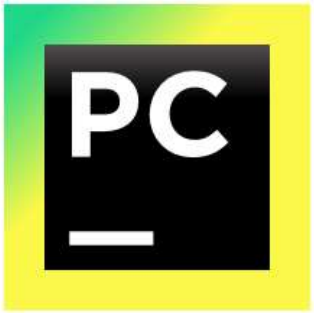
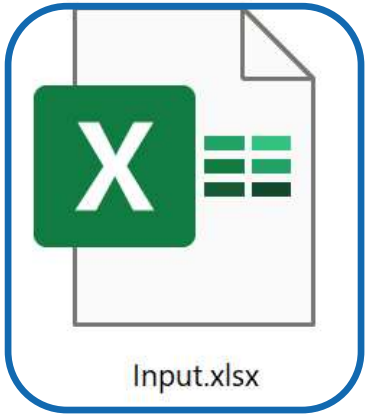
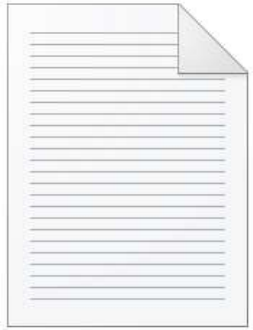
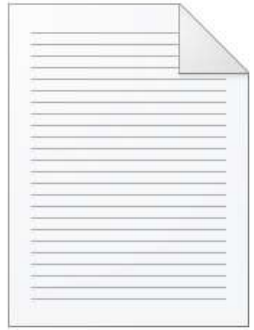

DecIDE.py


Input.xlsx


Output.xlsx


ReadMe.txt


requirements.txt

Check or manual feature input
- If you added the DIPPR files, this is automatically entered
- Otherwise, enter the features on your own

E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
N	countPro	BPmaxE	BPmaxP	BPminE	BPminP	MW_mainP	Cl	C	c	countReac	AddSidePro	stoichioH2	water	x_MP
en in the nts per ct	*Number of products in the reaction stoichiometry*	*Normal boiling point of the reactant with the highest boiling point*	*Normal boiling point of the product with the highest boiling point*	*Normal boiling point of the reactant with the lowest boiling point*	*Normal boiling point of the product with the lowest boiling point*	*Molecular weight of main product*	*Mole of chlorine atoms in the reactants per mole of product*	*Mole of reactant carbon atoms that are aliphatic (not part of an aromatic ring structure) per*	*Mole of reactant carbon atoms that are part of an aromatic ring structure per mole of*	*Number of reactants in the reaction stoichiometry*	*Expected occurrence of additional side products from possible side reactions. '0' = no, '1' = yes*	*Mole of H2 required as reactants per mole of product*	*Mole of water formed in the reaction per mole of product*	*molar fraction of main product : Mole of main product / mole of all products of the reaction*
nol]	[-]	[K]	[K]	[K]	[K]	[g/mol]	[mol/mol]	[mol/mol]	[mol/mol]	[-]	[-]	[mol/mol]	[mol/mol]	[mol/mol]
	3	351,44	373,15	351,44	20,268	54,09044	0	4	0	1	0	-1	2	0,25
	2	351,44	373,15	90,188	294,15	44,05256	0	2	0	2	0	0	1	0,5

Check or manual feature input

E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
N	countPro	BPmaxE	BPmaxP	BPminE	BPminP	MW_mainP	Cl	C	c	countReac	AddSidePro	stoichioH2	water	x_MP
en in the nts per ct	*Number of products in the reaction stoichiometry*	*Normal boiling point of the reactant with the highest boiling point*	*Normal boiling point of the product with the highest boiling point*	*Normal boiling point of the reactant with the lowest boiling point*	*Normal boiling point of the product with the lowest boiling point*	*Molecular weight of main product*	*Mole of chlorine atoms in the reactants per mole of product*	*Mole of reactant carbon atoms that are aliphatic (not part of an aromatic ring structure) per*	*Mole of reactant carbon atoms that are part of an aromatic ring structure per mole of*	*Number of reactants in the reaction stoichiometry*	*Expected occurrence of additional side products from possible side reactions. '0' = no, '1' = yes*	*Mole of H2 required as reactants per mole of product*	*Mole of water formed in the reaction per mole of product*	*molar fraction of main product : Mole of main product / mole of all products of the reaction*
nol]	[-]	[K]	[K]	[K]	[K]	[g/mol]	[mol/mol]	[mol/mol]	[mol/mol]	[-]	[-]	[mol/mol]	[mol/mol]	[mol/mol]
	3	351,44	373,15	351,44	20,268	54,09044	0	4	0	1	0	-1	2	0,25
	2	351,44	373,15	90,188	294,15	44,05256	0	2	0	2	0	0	1	0,5

Find the decision tree results here: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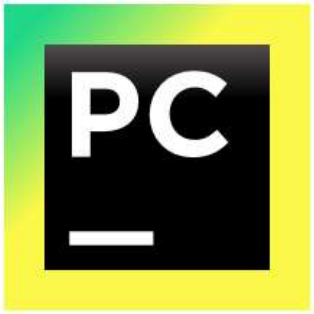
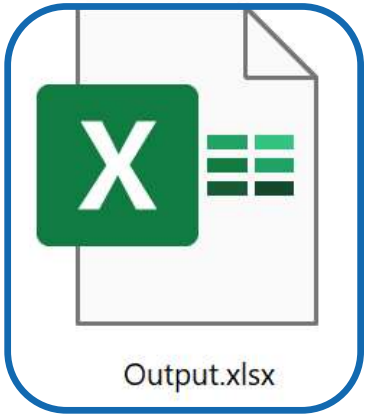
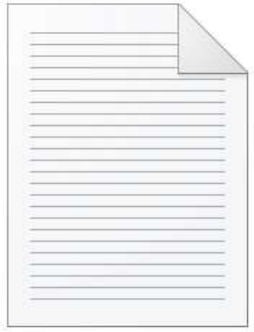
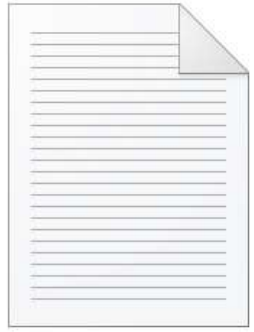

DecIDE.py


Input.xlsx


Output.xlsx


ReadMe.txt


requirements.txt

Estimated outputs:
- value = estimated value, provided in the unit mentioned above

C	D	E	F	G	H	I	J	K	L
Direct Emissions [kgCO2eq]		Electricity [MJ]		Natural Gas [MJ]		Steam [MJ]		Cooling Water [m^3]	
value	mae	value	mae	value	mae	value	mae	value	mae
2,995575497	1,053137714	0,3968712	0,1480948	2,1962746	2,2011697	10,395017	6,3333492	0,0763604	0,0357183
0,202675296	0,648806331	0,3836964	0,740548	0	0,1608223	-3,2899679	9,1487839	0,5363792	0,2435987

Estimated outputs :
- value = estimated value, provided in the unit mentioned above
- mae = mean absolute error of all processes in this leaf of the decision tree; measure of expected uncertainty

$$\mathrm{MAE} = \frac{\sum_{i=1}^{n} |y_i - x_i|}{n} = \frac{\sum_{i=1}^{n} |e_i|}{n}.$$

C	D	E	F	G	H	I	J	K	L
Direct Emissions [kgCO2eq]		Electricity [MJ]		Natural Gas [MJ]		Steam [MJ]		Cooling Water [m^3]	
value	mae	value	mae	value	mae	value	mae	value	mae
2,995575497	1,053137714	0,3968712	0,1480948	2,1962746	2,2011697	10,395017	6,3333492	0,0763604	0,0357183
0,202675296	0,648806331	0,3836964	0,740548	0	0,1608223	-3,2899679	9,1487839	0,5363792	0,2435987