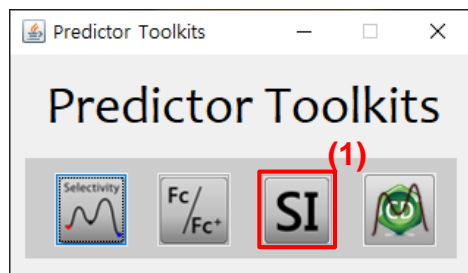


# Exporting Cartesian Coordinates



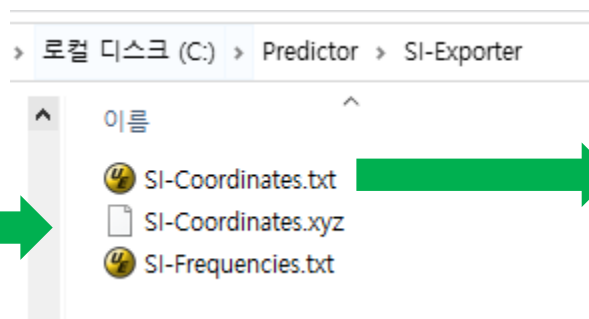
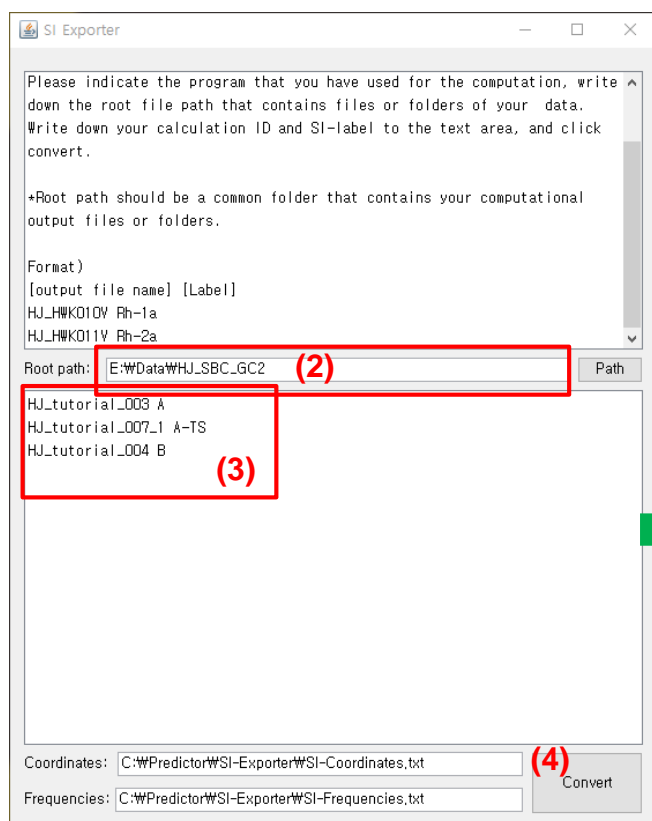
Step 0. Launch Predictor Toolkits.

Step 1. Click “SI-Exporter”.

Step 2. Fill in the proper root directory that contains your computational results.

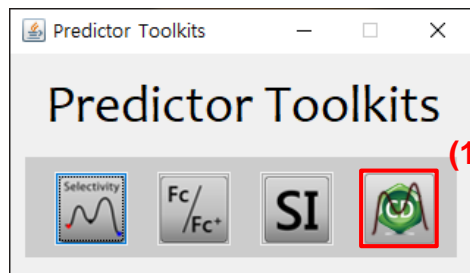
Step 3. Fill in the [output file name] [label] that will be seen in your combined xyz file.

Step 4. Check the directory for XYZ exportation, and click “Convert” button.



A			
Ir	1.430448	-0.262474	-1.172990
O	-0.862785	2.961974	-2.878110
H	-0.879564	0.902349	-4.726462
C	-1.258610	0.700070	-3.717778
C	-0.568270	1.634429	-2.799694
H	-3.065140	1.873489	-4.043415
C	-2.790896	0.879976	-3.670795
H	-0.958625	-0.311885	-3.447384
H	-3.226348	0.152110	-4.362109
N	0.298728	1.389056	-1.871198
C	-3.387701	0.671063	-2.265818
H	-2.984305	1.422282	-1.584285
H	-3.055510	-0.295434	-1.874937
Cl	-0.629769	-1.594610	-1.211001
Cl	1.802630	-0.730817	-3.545645
H	0.367100	-2.374571	1.299372
O	-0.107166	4.778429	-1.688846
A-TS			
Ir	0.690773	-0.192064	0.122364
O	0.804880	3.156862	0.415431
H	-1.437852	4.146922	0.942789
C	-1.975250	3.395842	0.161698
C	-0.258347	2.629955	0.076391
H	-2.651675	2.018135	1.411721
C	-2.762142	2.477763	0.426013
H	-1.702513	3.931983	-0.788750
H	-3.704866	3.039657	0.425214
N	-0.259013	1.382416	-0.516568
C	-2.811732	1.401199	-0.649030
H	-1.653001	1.040156	-0.706108
H	-2.928534	1.827055	-1.647786
Cl	-0.426430	0.127034	2.277445
B			
Ir	0.082871	-0.242082	-0.810403
Cl	0.305153	1.060023	-2.798351
Cl	0.778001	0.100288	2.182824

# Automatic generation of energy profiles



Step 0. Launch Predictor Toolkits.

Step 1. Click “Energy profile plotter”.

Step 2. Fill in the proper energy sequences.

→ Energy sequence should be in a row.

→ Multiple energy sequences will give multiple energy profiles

Step 3. Click “Generate” button.

