



main:606:execute  
100.00%  
(0.00%)  
1x

main:1366:saveEverything  
5.76%  
(0.00%)  
54x

model:581:enlarge  
93.47%  
(0.00%)  
107x

util:107:notify  
5.76%  
(0.46%)  
54x

runtime:234:call  
3.25%  
(0.62%)  
19322063x

model:804:processNewReactions  
31.56%  
(0.02%)  
32143x

react:116:reactAll  
61.35%  
(0.00%)  
54x

output:1347:update  
4.80%  
(0.00%)  
54x

adjlist:724:toAdjacencyList  
2.19%  
(1.23%)  
4343198x

model:488:makeNewReaction  
31.54%  
(0.00%)  
32193x

react:40:react  
61.35%  
(0.00%)  
54x

output:1311:saveOutput  
4.80%  
(0.00%)  
54x

model:307:makeNewSpecies  
31.50%  
(0.05%)  
110924x

util:153:map\_  
61.35%  
(0.00%)  
54x

output:45:saveOutputHTML  
4.80%  
(0.00%)  
108x

thermoengine:178:submit  
28.48%  
(0.00%)  
17789x

fallbacks:30:wrapper  
61.35%  
(0.00%)  
54x

draw:133:draw  
1.14%  
(0.02%)  
17719x

environment:993:render  
3.52%  
(0.00%)  
108x

util:156:submit\_  
28.48%  
(0.00%)  
17789x

~:0:<map>  
61.52%  
(0.17%)  
2708272x

surfaces:576:write\_to\_png  
0.91%  
(0.91%)  
17719x

~:0:<method 'join' of 'unicode' objects>  
3.52%  
(0.03%)  
9313x

thermoengine:160:evaluator  
28.48%  
(0.02%)  
17789x

util:110:\_\_\_call\_\_  
61.35%  
(0.00%)  
47904x

thermoengine:118:generateThermoData  
28.44%  
(0.00%)  
17789x

react:66:reactSpecies  
61.35%  
(0.02%)  
47904x

thermo:1103:getThermoData  
28.35%  
(0.47%)  
22070x

database:461:generate\_reactions\_from\_families  
60.63%  
(0.01%)  
47904x

thermo:1564:getThermoDataFromGroups  
27.39%  
(0.01%)  
17645x

thermo:1335:getThermoDataForSurfaceSpecies  
3.47%  
(0.07%)  
3863x

family:1658:addReverseAttribute  
3.43%  
(0.00%)  
2344x

thermo:1784:estimateThermoViaGroupAdditivity  
27.23%  
(0.00%)  
71377x

database:541:react\_molecules  
1.41%  
(0.01%)  
101976x

common:231:find\_degenerate\_reactions  
55.66%  
(10.28%)  
66672x

thermo:1693:estimateRadicalThermoViaHBI  
26.79%  
(0.22%)  
139487x

family:1624:generateReactions  
1.40%  
(0.03%)  
5608680x

family:1731:calculateDegeneracy  
23.55%  
(0.00%)  
16424x

thermo:1806:computeGroupAdditivityThermo  
24.48%  
(0.44%)  
71377x

family:1801:\_\_\_generateReactions  
25.44%  
(11.52%)  
10319079x

thermo:1910:\_\_\_addPolycyclicCorrectionThermoData  
19.51%  
(0.00%)  
60650x

thermo:2165:\_\_\_addGroupThermoData  
5.57%  
(0.07%)  
14085730x

family:1501:\_\_\_generatoProductStructures  
4.66%  
(0.02%)  
1524230x

common:154:ensure\_species  
24.89%  
(15.41%)  
831929x

thermo:1940:\_\_\_addPolyRingCorrectionThermoDataFromHeuristic  
5.82%  
(0.01%)  
11871x

~:0:<method 'format' of 'str' objects>  
1.86%  
(1.69%)  
1158899173x

model:238:checkForExistingSpecies  
2.91%  
(2.05%)  
110924x

family:1215:applyRecipe  
4.17%  
(1.93%)  
1483781x

filtration:53:filter\_structures  
1.20%  
(0.01%)  
930576x

thermo:1996:getBicyclicCorrectionThermoDataFromHeuristic  
8.82%  
(0.05%)  
52482x

Graph:45:from\_edges  
5.30%  
(0.53%)  
31346334x

Graph:81:add\_edge  
4.68%  
(2.45%)  
790611787x

filtration:390:mark\_unreactive\_structures  
1.05%  
(0.32%)  
930576x

thermo:2070:\_\_\_addRingCorrectionThermoDataFromTree  
19.89%  
(0.03%)  
414906x

Graph:75:\_\_\_add\_or\_get\_node\_index  
1.49%  
(1.27%)  
1581223574x

copy:145:deepcopy  
15.86%  
(6.06%)  
2429363888x

copy:267:keep\_alive  
5.53%  
(4.96%)  
2425392867x

base:989:descendTree  
24.30%  
(0.48%)  
41812437x

~:0:<method 'get' of 'dict' objects>  
0.83%  
(0.83%)  
4891453336x

copy:253:deepcopy\_dict  
11.99%  
(1.72%)  
806759381x

base:908:matchNodeToStructure  
23.78%  
(22.98%)  
426012546x