Compound	Method	Solvent	Simtime	repeats
22	cMD, GaMD, aMD	H_2O	2000	1

hash = $f(\{parameters\})$

hash	Compound	method	Solvent	Simtime	repeat
ea902b72	22	GaMD	H_2O	2000	1
734cdc50	22	cMD	H_2O	2000	1
bb375067	22	aMD	H_2O	2000	1