This article describes how to use PyRx to run AutoDock Vina jobs on Amazon Web Services (AWS) High-Performance Computing (HPC) cluster. If you don't have access to a local HPC cluster, this is a good option for running jobs since you will not pay large upfront cost for HPC cluster but can use pay-as-you-go approach instead. To get started, follow step 1 in Launch an HPC Cluster to get your key pair. Then follow step 2 to launch and configure your HPC cluster. Instead of using Computational Fluid Dynamics (CFD) job template download pyrx-cfncluster.cfn.txt and use Browse button to upload this template to Amazon S3.

Note that next time you lunch a cluster, you don't need to upload this template again. You can find this uploaded template in your Amazon S3 bucket and specify template URL instead. The following are major differences between this template and CFD job template:
- We use c4.xlarge for ComputeInstanceType instead of c4.8xlarge. Default bid per spot instance is correspondingly different. Check Amazon EC2 Spot Instances Pricing in the region you are launching HPC cluster and change default bid as needed. c4.xlarge is using 4 vCPU and 7.5 Mem (GiB) which is fine for most Vina jobs. You can change ComputeInstanceType to c4.2xlarge or higher as needed.

- InitialQueueSize is 1 and MaxQueueSize is 10 in our template compared to 2 and 2 correspondingly in CFD job template. You can read cfnccluster documentation to learn more about this parameters.

- We don't run PostInstallScript.

Continue with the rest of the steps 2 c to f in Launch an HPC Cluster. When the cluster is about to complete, in PyRx, Vina Start page click on Remote (HPC/AWS) as shown in the image below. Enter Key pair from Step 1 and MasterPublicIP for Host Name or IP address from Step 2.
Click OK and follow Vina Wizard. PyRx uploads all the files needed to AWS, lunches Vina jobs, waits for the jobs to finish and downloads the results. When all results are downloaded, terminate your cluster following Step 5 in Launch an HPC Cluster.