Commands to Run Vina for Virtual Screening in Linux Environment

Step-1: Update and Upgrade your System

```
sudo apt-get update
sudo apt-get upgrade
```

Step-2: Install Open Babel in your System

```
sudo apt install openbabel
```

Step-3: Install Vina in your System

```
Sudo apt install autodock-vina
```

Step-4: Splitting of Single Ligands file into Multiple

```
obabel -isdf ligand.sdf -osdf -O *.sdf –split
```

Note: Ligand name in the above command may be different in your case.

Step-5: Ligands Energy Minimization Using Openbabel

```
obminimize -ff MMFF94 -n 1000 *.sdf
```

Step-6: Conversion of Ligand Formate into pdbqt

```
obabel -isdf *.sdf -opdbqt -O*.pdbqt
```

Step-7: Writing of Ligands Names in .txt file

```
ls >ligand.txt
```

Step-7: Writing of Ligands Names in .txt file

```
perl Vina_linux.pl
```

Step-8: Combining all .log Files

```
tail -n11 *.log > results_log.txt
```