Table S2: Comparative molecular docking studies of top-ranked virtual compounds against two selected targets 1MQ4 (Prostate Cancer) and 4UYA (Renal Cancer)

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| --- | --- | --- | --- | --- |
| **PDB ID** | **2D Structures and virtual compound number** | **Interacting residues** | **Binding Energy (kcal/mol)** | **Molecular docking software/tool** |
| 1MQ4 | C:\Users\ADMIN\Desktop\VM_8.tif  RVC-8 | H-bond interaction with Lys141, Val147, Asn261, Asp256 | -7.9 | MOE |
| 4UYA | C:\Users\ADMIN\Desktop\VM7.tif  RVC-7 | H-bond interaction with Lys151 and Asp289 | -8.2 | MOE |
| 1MQ4 | C:\Users\ADMIN\Desktop\VM_13.tif  RVC-13 | H-bond interaction with Glu185, Asp274 | -10.2 | Cresset-Flare |
| 4UYA | C:\Users\ADMIN\Desktop\VM_13.tif  RVC-13 | H-bond interaction with Asn268, Lys151 | -9.4 | Cresset-Flare |
| 1MQ4 | C:\Users\ADMIN\Desktop\VM7.tif  RVC-7 | H-bond interaction with Lys258, Gly291, Asp256 and Trp277 | -7.8 | Auto Dock Vina |
| 4UYA | C:\Users\ADMIN\Desktop\VM4.tif  RVC-4 | H-bond interaction with Asp125 and Glu121 | 7.7 | Auto Dock Vina |
| 1MQ4 | C:\Users\ADMIN\Desktop\VM_19.tif  RVC-19 | H-bond interaction with Ala213, Lys162 and Ala160 | -6.2 | GLIDE |
| 4UYA | C:\Users\ADMIN\Desktop\VM_16.tif  RVC-16 | H-bond interaction with Glu201, Ala203, Lys151, Asn268, Lys265 and Thr288 | -8.4 | GLIDE |