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| **Table S1. The source of 3D structures of TTK and three interacting drugs** | | | |
| Synonyms | Name | Source | Link |
| Dual specificity protein kinase TTK | TTK | Alphafold | https://alphafold.ebi.ac.uk/entry/P33981 |
| Empesertib | BAY-1161909 | PubChem | https://pubchem.ncbi.nlm.nih.gov/compound/71599640 |
| Benzamide, N-cyclopropyl-4-[6-(2,3-difluoro-4-methoxyphenoxy)-8-[(3,3,3-trifluoropropyl)amino]imidazo[1,2-b]pyridazin-3-yl]-2-methyl- | BAY-1217389 | PubChem | https://pubchem.ncbi.nlm.nih.gov/compound/78320750 |
| Hesperadine | Hesperadin | PubChem | https://pubchem.ncbi.nlm.nih.gov/compound/135421442 |