**Identification of Novel Mutant (R132H) Isocitrate Dehydrogenase 1 Inhibitors for Glioma Therapy**

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**Table Legends**

**Table S1** The PDB IDs of mIDH1 protein along with the resolution

**Table S2** Glide docking score and energy of lead molecules

**Table S3** The biological activity spectrum prediction using PASS

**Table S1** ThePDB IDs of mIDH1 protein along with their resolutions.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| S.No | PDB Codes | Resolution(Å) | Mutational positions | Complex |
|  | 4I3K | 3.31 | R132H | 1-hydroxy-6-(4-hydroxybenzyl)-4methylpyridin-2(1H)-one |
|  | 4I3L | 3.29 | R132H | 1-hydroxy-6-(4-hydroxybenzyl)-4-methylpyridin-2(1H)-one |
|  | 4UMX | 1.88 | R132H | Cpd-1 |
|  | 4XS3 | 3.29 | R132H, R132C | 2-Thiahydantoin |
|  | 5L57 | 2.69 | R132H | Compound 13a |
|  | 5L58 | 3.04 | R132H | Compound 2 |
|  | 5LGE | 2.70 | R132H | BAY 1436032 |
|  | 5SUN | 2.48 | R132H | IDH146 |
|  | 5SVF | 2.34 | R132H | IDH125 |
|  | 5TQH | 2.20 | R132H | IDH889 |
|  | 6ADG | 3.00 | R132H | AG-881 |
|  | 6B0Z | 2.33 | R132H | IDH305 |
|  | 6IO0 | 2.20 | R132H | Compound A |
|  | 6O2Y | 2.80 | R132H | Compound 24 |
|  | 6O2Z | 2.50 | R132H | Compound 32 |
|  | 6Q6F | 3.30 | R132H | HMS101 |
|  | 6U4J | 2.11 | R132H | FT-2102 |
|  | 6VEI | 2.10 | R132H | AG-881 |
|  | 6VG0 | 2.66 | R132H | AGI-15056 |

**Table S2** Glide docking score and energy of lead molecules

|  |  |  |
| --- | --- | --- |
| S. No. | DrugBankIDs | XP Gscore (kcal/mol) |
|  | DB14650 | -9.964 |
|  | DB03310 | -9.861 |
|  | DB01632 | -9.386 |
|  | DB01698 | -8.769 |
|  | DB03147 | -8.634 |
|  | DB01076 | -7.302 |
|  | DB12010 | -7.147 |
|  | DB00157 | -6.995 |
|  | DB00521 | -6.943 |
|  | DB00368 | -6.780 |
|  | DB00968 | -6.681 |
|  | DB01250 | -6.655 |
|  | DB01001 | -6.623 |
|  | DB00355 | -6.604 |
|  | DB01235 | -6.565 |
|  | DB12107 | -6.447 |
|  | DB00642 | -6.431 |
|  | DB00114 | -6.380 |
|  | DB08976 | -6.355 |
|  | DB15694 | -6.248 |
|  | DB00439 | -6.230 |
|  | DB00456 | -6.163 |
|  | DB00987 | -6.143 |
|  | DB04868 | -6.141 |
|  | DB01102 | -6.074 |
|  | DB00183 | -6.028 |
|  | DB01399 | -6.018 |
|  | DB11796 | -5.997 |
|  | DB06707 | -5.992 |
|  | DB01064 | -5.985 |
|  | DB12789 | -5.973 |
|  | DB00861 | -5.939 |
|  | DB00900 | -5.922 |
|  | DB03209 | -5.918 |
|  | DB03209 | -5.918 |
|  | DB14075 | -5.911 |
|  | DB00293 | -5.899 |
|  | DB07565 | -5.893 |
|  | DB01098 | -5.874 |
|  | DB00492 | -5.854 |
|  | DB12001 | -5.828 |
|  | DB13874 | -5.793 |
|  | DB05016 | -5.770 |
|  | DB00229 | -5.752 |
|  | DB13751 | -5.744 |
|  | DB05018 | -5.720 |
|  | DB06441 | -5.718 |
|  | DB14975 | -5.630 |
|  | DB01326 | -5.624 |
|  | DB00651 | -5.594 |
|  | DB00238 | -5.588 |
|  | DB05039 | -5.577 |
|  | DB08905 | -5.538 |
|  | DB00430 | -5.496 |
|  | DB06769 | -5.480 |
|  | DB00610 | -5.477 |
|  | DB06590 | -5.454 |
|  | DB04880 | -5.443 |
|  | DB06211 | -5.433 |

**Table S3** The biological activity spectra prediction using PASS

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| S.No | Compounds | Pa | Pi | Predicted Activity |
| 1. | Vorasidenib | 0.521 | 0.065 | Antineoplastic |
|  |  | 0.157 | 0.116 | Antineoplastic (bladder cancer) |
|  |  | 0.241 | 0.021 | Antineoplastic (carcinoma) |
|  |  | 0.149 | 0.141 | Antineoplastic (endocrine cancer) |
|  |  | 0.388 | 0.042 | Antineoplastic (solid tumors) |
|  |  | 0.290 | 0.013 | Antineoplastic (squamous cell carcinoma) |
| 2. | DB12001 | 0.586 | 0.048 | Antineoplastic |
|  |  | 0.147 | 0.140 | Antineoplastic (breast cancer) |
|  |  | 0.295 | 0.034 | Antineoplastic (colon cancer) |
|  |  | 0.308 | 0.034 | Antineoplastic (colorectal cancer) |
|  |  | 0.283 | 0.097 | Antineoplastic (multiple myeloma) |
|  |  | 0.316 | 0.202 | Antineoplastic (non-Hodgkin's lymphoma) |
|  |  | 0.283 | 0.104 | Antineoplastic (solid tumors) |