|  |  |  |  |
| --- | --- | --- | --- |
| S.No | Reference Drug Name | Structural Similarity | Predicted IC50 value (µmol) |
| 1 | Alectinib | 3-amino-6,6-dimethyl-9-[4-(oxetan-3-yl)piperazin-1-yl]-5H-benzo[b]carbazol-11-one | 0.758705 |
| 2 | Amuvatinib | 3-(1,3-Benzodioxol-5-yl)-1-[4-([1]benzofuro[3,2-d]pyrimidin-4-yl)piperazin-1-yl]propane-1-thione;methanesulfonic acid | 1.804693 |
| 3 | AST-1306 | [1-[[4-[3-Chloro-4-[(3-fluorophenyl)methoxy]anilino]quinazolin-6-yl]amino]-2-(2-fluorobutoxycarbonylamino)-1-oxopropan-2-yl] acetate | 0.509847 |
| 4 | Axitinib | N-[5-(hydroxyamino)-5-oxopentyl]-2-[[3-(2-pyridin-2-ylethenyl)-1H-indazol-6-yl]sulfanyl]benzamide | 1.010532 |
| 5 | AZD1332 | 5-Chloro-N2-[(1S)-1-(5-fluoropyridin-2-yl)ethyl]-N4-(5-isopropoxy-1H-pyrazol-3-yl)pyrimidine-2,4-diamine phosphate | 1.946533 |
| 6 | AZD4547 | 1-chloro-N,N,2-trimethylprop-1-en-1-amine;N-[5-[2-(3,5-dimethoxyphenyl)ethyl]-1H-pyrazol-3-yl]-3-methoxybenzamide | 1.443234 |
| 7 | AZD6094 | 3-(Imidazo[1,2-b]pyridazin-6-ylmethyl)-5-(1-methylpyrazol-4-yl)triazolo[4,5-b]pyrazine | 2.287226 |
| 8 | AZD8931 | 6-[4-(3-chloroanilino)-7-methoxyquinazolin-6-yl]oxy-N-hydroxyhexanamide | 0.66 |
| 9 | BIBF-1120 | methyl 3-[N-[4-[(3-aminopropylamino) methyl]phenyl]-C-phenylcarbonimidoyl]-2-hydroxy-1H-indole-6-carboxylate | 1.385818 |
| 10 | BMS-754807 | N-[1-[4-[(5-cyclopropyl-1H-pyrazol-3-yl)amino]pyrrolo[2,1-f][1,2,4]triazin-2-yl]piperidin-4-yl]acetamide | 1.224906 |
| 11 | Cabozantinib | 4-(6,7-dimethoxyquinolin-4-yl)oxy-N-[3-(4-fluorophenyl)propyl]aniline | 1.231128 |
| 12 | CI-1033 | (Z)-N-[4-(3-chloro-4-fluoroanilino)-7-(difluoromethoxy)quinazolin-6-yl]-4-(dimethylamino)but-2-enamide | 1.073408 |
| 13 | Crizotinib | 3-Phenylmethoxy-5-(1-piperidin-4-ylpyrazol-4-yl)pyridin-2-amine | 1.647109 |
| 14 | Dasatinib | N-(2-chloro-6-methylphenyl)-2-[[6-[4-(2-hydroxyethyl)piperazin-1-yl]-2-methylpyrimidin-4-yl]amino]-1,3-thiazole-5-carboxamide;sulfuric acid | 1.062769 |
| 15 | Foretinib | N-[4-[7-(3-bromopropoxy)-6-methoxyquinolin-4-yl]oxy-3-fluorophenyl]-1-formylcyclopropane-1-carboxamide | 0.802407 |
| 16 | GSK 1904529A | N-(2,6-difluorophenyl)-3-{3-[2-({5-methyl-2-(methyloxy)-4-[4-(methylsulfonyl)-1-piperazinyl]phenyl}amino)-4 pyrimidinyl]imidazo[1,2-a]pyridin-2-yl}benzamide | 1.062241 |
| 17 | GW2580 | 2,4-Diamino-5-[3,4-dimethoxy-5-(2-propynyloxy)benzyl]pyrimidine | 1.320202 |
| 18 | GW441756 | (3Z)-3-ethylidene-1H-pyrrolo[3,2-b]pyridin-2-one;1-methylindole | 1.021878 |
| 19 | JNJ38877605 | 6-[Difluoro-(6-iodo-[1,2,4]triazolo[4,3-b]pyridazin-3-yl)methyl]quinoline | 0.908253 |
| 20 | Kobe 2602 | 1-(4-Ethylphenyl)-3-[2-nitro-4-(trifluoromethyl)anilino]thiourea | 1.096508 |
| 21 | lapatinib | Methyl 6-[[5-[4-[3-chloro-4-[(3-fluorophenyl)methoxy]anilino]quinazolin-6-yl]furan-2-yl]methylamino]hexanoate | 0.739111 |
| 22 | Linifanib | 1-[4-(3-amino-1H-indazol-4-yl)phenyl]-3-(2-fluoro-5-methylphenyl)-1-(2-hydroxyethyl)urea | 1.442908 |
| 23 | Masitinib | 4-(2-aminophenyl)-1-N-[4-methyl-3-[(4-pyridin-3-yl-1,3-thiazol-2-yl)amino]phenyl]cyclohexa-1,5-diene-1,4-dicarboxamide | 1.882307 |
| 24 | Motesanib | N-(4-pentylphenyl)-2-(pyridin-4-ylmethylamino)pyridine-3-carboxamide | 0.988261 |
| 25 | NVP-TAE684 | 5-chloro-2-N-[2-methoxy-4-(4-piperazin-4-ium-1-ylpiperidin-1-yl)phenyl]-4-N-(2-propan-2-ylsulfonylphenyl)pyrimidine-2,4-diamine;2,2,2-trifluoroacetate | 0.907894 |
| 26 | OSI-930 | 3-(pyridin-4-ylmethylamino)-N-[4-(trifluoromethoxy)phenyl]thiophene-2-carboxamide | 1.790038 |
| 27 | Pazopanib | 3-[4-[[4-[(2,3-dimethylindazol-6-yl)-methylamino]pyrimidin-2-yl]amino]phenyl]-N-methylpropane-1-sulfinamide | 1.30786 |
| 28 | PD173074 | tert-butyl N-[N'-[2-[amino-[(Z)-2-amino-3-[[7-(tert-butylcarbamoylamino)-6-(3,5-dimethoxyphenyl)pyrido[2,3-d]pyrimidin-2-yl]amino]prop-1-enyl]amino]ethyl]-N-[(2-methylpropan-2-yl)oxycarbonyl]carbamimidoyl]carbamate | 1.104513 |
| 29 | PF-00299804 | N-[4-(3-chloro-4-fluoroanilino)-7-(difluoromethoxy)quinazolin-6-yl]acetamide | 1.065045 |
| 30 | PHA-665752 | 5-[5-(2,6-Dichloro-phenylmethanesulfonyl)-2-oxo-1,2-dihydro-indol-(3Z)-ylidenemethyl]-2,4-dimethyl-1H-pyrrole-3-carboxylic acid amide | 1.004722 |
| 31 | Quizartinib | 1-[4-(6-Methoxyimidazo[2,1-b][1,3]benzothiazol-2-yl)phenyl]-3-(3-methyl-1,2-oxazol-5-yl)urea | 1.197091 |
| 32 | SB505124 | 4-(1,3-benzodioxol-5-yl)-5-(6-methylpyridin-2-yl)-1H-imidazol-2-amine | 1.402854 |
| 33 | SB52334 | Ethane;2-methylpyridine-3-carboxylic acid | 1.944159 |
| 34 | Sorafenib | 4-[4-[[[[4-Chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-3-fluorophenoxy]-N-methyl-2-pyridinecarboxamide hydrate | 2.10531 |
| 35 | SU11274 | tert-butyl 4-[5-[(Z)-[5-[(3-chlorophenyl)-methylsulfamoyl]-2-oxo-1H-indol-3-ylidene]methyl]-2,4-dimethyl-1H-pyrrole-3-carbonyl]piperazine-1-carboxylate | 1.006986 |
| 36 | Sunitinib | N-[2-(diethylamino)ethyl]-5-[1-(5-fluoro-2-oxo-1,3-dihydroindol-3-yl)propyl]-2,4-dimethyl-1H-pyrrole-3-carboxamide | 1.526341 |
| 37 | Tivozanib | 1-[4-(6,7-Dimethoxyquinolin-4-yl)oxyphenyl]-3-(5-methyl-1,2-oxazol-3-yl)urea | 1.260934 |

Table 2 : Tabular column representing the top Structural similarities of each Drug molecule