Ranking of 6666 + 6677

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12 Apr 2022

# Location of 6666 and 6677

Tables are filtered for Atom as the phosphate only.

## Rank

**Table** : Top 5 scoring RMSD MAP

| **drug** | **compound** | **alphavalue** | **nl** | **rank** | **RMSD\_MAP** |
| --- | --- | --- | --- | --- | --- |
| Phosphate | Compound\_1 | 3.459 | 6666 | 4 | 0.02802 |
| 3.600 | 6666 | 4 | 0.02802 |
| 3.800 | 6666 | 4 | 0.02802 |
| Phosphonate | 3.459 | 6666 | 3 | 0.02979 |
| 3.600 | 6666 | 3 | 0.02979 |
| 3.800 | 6666 | 3 | 0.02979 |
| Compound\_2 | 3.459 | 6666 | 4 | 0.03067 |
| 3.600 | 6666 | 4 | 0.03067 |
| 3.800 | 6666 | 4 | 0.03067 |
| Phosphoroamidate | Compound\_3 | 3.459 | 6666 | 15 | 0.03144 |
| 3.600 | 6666 | 15 | 0.03144 |
| 3.800 | 6666 | 15 | 0.03144 |
| Phosphorodiamidate | Compound\_1 | 3.459 | 6666 | 41 | 0.03244 |
| 3.600 | 6666 | 41 | 0.03244 |
| 3.800 | 6666 | 41 | 0.03244 |
| Phosphinate | Compound\_2 | 3.459 | 6666 | 35 | 0.03297 |
| 3.600 | 6666 | 35 | 0.03297 |
| 3.800 | 6666 | 35 | 0.03297 |
| Phosphonate | Compound\_3 | 3.459 | 6666 | 42 | 0.03302 |
| 3.600 | 6666 | 42 | 0.03302 |
| 3.800 | 6666 | 42 | 0.03302 |
| Phosphinite | Compound\_1 | 3.459 | 6666 | 204 | 0.03336 |
| 3.600 | 6666 | 204 | 0.03336 |
| 3.800 | 6666 | 204 | 0.03336 |
| Phosphonite | Compound\_3 | 3.459 | 6666 | 167 | 0.03359 |
| 3.600 | 6666 | 167 | 0.03359 |
| 3.800 | 6666 | 167 | 0.03359 |
| Phosphate | 3.459 | 6666 | 13 | 0.03401 |
| 3.800 | 6666 | 13 | 0.03401 |
| Phosphonamidite | 3.459 | 6666 | 187 | 0.03402 |
| 3.600 | 6666 | 187 | 0.03402 |
| 3.800 | 6666 | 187 | 0.03402 |
| Phosphinite | Compound\_2 | 3.459 | 6666 | 206 | 0.03450 |
| 3.600 | 6666 | 206 | 0.03450 |
| 3.800 | 6666 | 206 | 0.03450 |
| Phosphine | 3.459 | 6666 | 237 | 0.03507 |
| 3.600 | 6666 | 237 | 0.03507 |
| 3.800 | 6666 | 237 | 0.03507 |
| Phosphonite | 3.459 | 6666 | 185 | 0.03518 |
| 3.600 | 6666 | 185 | 0.03518 |
| 3.800 | 6666 | 185 | 0.03518 |
| Phosphinamidate | Compound\_3 | 3.459 | 6666 | 32 | 0.03524 |
| 3.600 | 6666 | 32 | 0.03524 |
| 3.800 | 6666 | 32 | 0.03524 |
| Compound\_1 | 3.459 | 6666 | 26 | 0.03566 |
| 3.600 | 6666 | 26 | 0.03566 |
| 3.800 | 6666 | 26 | 0.03566 |
| Phosphinate | 3.459 | 6666 | 5 | 0.03569 |
| 3.600 | 6666 | 5 | 0.03569 |
| 3.800 | 6666 | 5 | 0.03569 |
| Phosphine | 3.459 | 6666 | 243 | 0.03575 |
| 3.600 | 6666 | 243 | 0.03575 |
| 3.800 | 6666 | 243 | 0.03575 |
| Phosphite | Compound\_3 | 3.459 | 6666 | 192 | 0.03594 |
| 3.600 | 6666 | 192 | 0.03594 |
| 3.800 | 6666 | 192 | 0.03594 |
| Phosphorodiamidtite | Compound\_2 | 3.459 | 6666 | 171 | 0.03624 |
| 3.600 | 6666 | 151 | 0.03624 |
| 3.800 | 6666 | 171 | 0.03624 |
| PhosphineOxide | Compound\_1 | 3.459 | 6666 | 32 | 0.03631 |
| 3.600 | 6666 | 32 | 0.03631 |
| 3.800 | 6666 | 32 | 0.03631 |
| Phosphoroamidate | 3.459 | 6666 | 16 | 0.03654 |
| 3.600 | 6666 | 16 | 0.03654 |
| 3.800 | 6666 | 16 | 0.03654 |
| Phosphondiamidate | 3.459 | 6666 | 47 | 0.03666 |
| 3.600 | 6666 | 47 | 0.03666 |
| 3.800 | 6666 | 47 | 0.03666 |
| Phosphorodiamidate | Compound\_2 | 3.459 | 6666 | 25 | 0.03675 |
| 3.600 | 6666 | 25 | 0.03675 |
| 3.800 | 6666 | 25 | 0.03675 |
| PhosphineOxide | Compound\_3 | 3.459 | 6666 | 64 | 0.03695 |
| 3.600 | 6666 | 64 | 0.03695 |
| 3.800 | 6666 | 64 | 0.03695 |
| Phosphondiamidate | Compound\_2 | 3.600 | 6666 | 24 | 0.03732 |
| 3.800 | 6666 | 24 | 0.03732 |
| 3.459 | 6666 | 24 | 0.03733 |
| Phosphorodiamidate | Compound\_3 | 6666 | 33 | 0.03742 |
| 3.600 | 6666 | 33 | 0.03742 |
| 3.800 | 6666 | 33 | 0.03742 |
| Phosphonamidite | Compound\_1 | 3.459 | 6666 | 191 | 0.03810 |
| 3.600 | 6666 | 191 | 0.03810 |
| 3.800 | 6666 | 191 | 0.03810 |
| Phosphate | Compound\_2 | 3.459 | 6666 | 6 | 0.03816 |
| 3.600 | 6666 | 6 | 0.03816 |
| 3.800 | 6666 | 6 | 0.03816 |
| Phosphoamidite | Compound\_3 | 3.459 | 6666 | 166 | 0.03826 |
| 3.600 | 6666 | 166 | 0.03826 |
| 3.800 | 6666 | 166 | 0.03826 |
| Phosphonodiamidite | 3.459 | 6666 | 205 | 0.03855 |
| 3.600 | 6666 | 205 | 0.03855 |
| 3.800 | 6666 | 205 | 0.03855 |
| Phosphite | Compound\_1 | 3.459 | 6666 | 158 | 0.03870 |
| 3.600 | 6666 | 158 | 0.03870 |
| 3.800 | 6666 | 158 | 0.03870 |
| Phosphorotriamidite | 3.459 | 6666 | 212 | 0.03925 |
| 3.600 | 6666 | 212 | 0.03925 |
| 3.800 | 6666 | 212 | 0.03925 |
| Phosphite | Compound\_2 | 3.459 | 6666 | 162 | 0.03942 |
| 3.600 | 6666 | 162 | 0.03942 |
| 3.800 | 6666 | 162 | 0.03942 |
| Phosphoamidite | 3.459 | 6666 | 188 | 0.03967 |
| 3.600 | 6666 | 188 | 0.03967 |
| 3.800 | 6666 | 188 | 0.03967 |
| Phosphorotriamidate | Compound\_3 | 3.459 | 6666 | 39 | 0.03974 |
| 3.800 | 6666 | 39 | 0.03974 |
| Phosphinite | 3.459 | 6666 | 231 | 0.04037 |
| 3.600 | 6666 | 231 | 0.04037 |
| 3.800 | 6666 | 231 | 0.04037 |
| Phosphonite | Compound\_1 | 3.459 | 6666 | 179 | 0.04037 |
| 3.600 | 6666 | 179 | 0.04037 |
| 3.800 | 6666 | 179 | 0.04037 |
| Phosphine | Compound\_3 | 3.459 | 6666 | 260 | 0.04038 |
| 3.600 | 6666 | 260 | 0.04038 |
| 3.800 | 6666 | 260 | 0.04038 |
| Phosphoamidite | Compound\_1 | 3.459 | 6666 | 173 | 0.04046 |
| 3.600 | 6666 | 173 | 0.04046 |
| 3.800 | 6666 | 173 | 0.04046 |
| Phosphonamidite | Compound\_2 | 3.459 | 6666 | 209 | 0.04060 |
| 3.600 | 6666 | 209 | 0.04060 |
| 3.800 | 6666 | 209 | 0.04060 |
| Phosphoroamidate | 3.459 | 6666 | 11 | 0.04104 |
| 3.600 | 6666 | 11 | 0.04104 |
| Phosphorodiamidtite | Compound\_3 | 3.459 | 6666 | 189 | 0.04168 |
| 3.600 | 6666 | 189 | 0.04168 |
| 3.800 | 6666 | 189 | 0.04168 |
| Phosphonodiamidite | Compound\_2 | 3.459 | 6666 | 215 | 0.04245 |
| 3.600 | 6666 | 215 | 0.04245 |
| 3.800 | 6666 | 215 | 0.04245 |
| Phosphinate | Compound\_3 | 3.459 | 6666 | 19 | 0.04252 |
| 3.600 | 6666 | 19 | 0.04252 |
| 3.800 | 6666 | 19 | 0.04252 |
| Phosphorotriamidate | Compound\_2 | 3.459 | 6666 | 35 | 0.04273 |
| 3.600 | 6666 | 35 | 0.04273 |
| 3.800 | 6666 | 35 | 0.04273 |
| PhosphineOxide | 3.459 | 6666 | 128 | 0.04301 |
| 3.600 | 6666 | 128 | 0.04301 |
| 3.800 | 6666 | 128 | 0.04301 |
| Phosphondiamidate | Compound\_3 | 3.459 | 6666 | 29 | 0.04321 |
| 3.600 | 6666 | 29 | 0.04321 |
| 3.800 | 6666 | 29 | 0.04321 |
| Phosphorotriamidite | 3.459 | 6666 | 227 | 0.04366 |
| 3.600 | 6666 | 227 | 0.04366 |
| 3.800 | 6666 | 227 | 0.04366 |
| Phosphinamidate | Compound\_2 | 3.459 | 6666 | 53 | 0.04500 |
| 3.600 | 6666 | 53 | 0.04500 |
| 3.800 | 6666 | 53 | 0.04500 |
| Phosphorotriamidate | Compound\_1 | 3.600 | 6666 | 140 | 0.04503 |
| 3.800 | 6666 | 161 | 0.04517 |
| 3.459 | 6666 | 163 | 0.04518 |
| Phosphorodiamidtite | 6666 | 190 | 0.04647 |
| 3.600 | 6666 | 190 | 0.04647 |
| 3.800 | 6666 | 190 | 0.04647 |
| Phosphorotriamidite | Compound\_2 | 3.459 | 6666 | 217 | 0.04718 |
| 3.600 | 6666 | 217 | 0.04718 |
| 3.800 | 6666 | 217 | 0.04718 |
| Phosphonodiamidite | Compound\_1 | 3.459 | 6666 | 211 | 0.04786 |
| 3.600 | 6666 | 211 | 0.04786 |
| 3.800 | 6666 | 211 | 0.04786 |