Ranking of 6666 + 6677

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# 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 |
| 3.459 | 6677 | 18 | 0.02821 |
| 3.600 | 6677 | 18 | 0.02821 |
| 3.800 | 6677 | 18 | 0.02821 |
| phosphonate | 3.459 | 6666 | 3 | 0.02979 |
| 3.600 | 6666 | 3 | 0.02979 |
| 3.800 | 6666 | 3 | 0.02979 |
| 3.459 | 6677 | 34 | 0.03000 |
| 3.600 | 6677 | 34 | 0.03000 |
| 3.800 | 6677 | 34 | 0.03000 |
| Compound\_2 | 3.459 | 6666 | 4 | 0.03067 |
| 3.600 | 6666 | 4 | 0.03067 |
| 3.800 | 6666 | 4 | 0.03067 |
| 3.459 | 6677 | 33 | 0.03088 |
| 3.600 | 6677 | 33 | 0.03088 |
| 3.800 | 6677 | 33 | 0.03088 |
| phosphoroamidate | Compound\_3 | 3.459 | 6666 | 15 | 0.03144 |
| 3.600 | 6666 | 15 | 0.03144 |
| 3.800 | 6666 | 15 | 0.03144 |
| 3.459 | 6677 | 15 | 0.03144 |
| 3.600 | 6677 | 15 | 0.03144 |
| 3.800 | 6677 | 15 | 0.03144 |
| phosphorodiamidate | Compound\_1 | 3.459 | 6677 | 34 | 0.03241 |
| 3.600 | 6677 | 34 | 0.03241 |
| 3.800 | 6677 | 34 | 0.03241 |
| 3.459 | 6666 | 42 | 0.03244 |
| 3.600 | 6666 | 42 | 0.03244 |
| 3.800 | 6666 | 42 | 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 | 6677 | 138 | 0.03302 |
| 3.600 | 6677 | 138 | 0.03302 |
| 3.800 | 6677 | 138 | 0.03302 |
| phosphinate | Compound\_2 | 3.459 | 6677 | 51 | 0.03305 |
| 3.600 | 6677 | 51 | 0.03305 |
| 3.800 | 6677 | 51 | 0.03305 |
| phosphonate | Compound\_3 | 3.459 | 6677 | 60 | 0.03308 |
| 3.600 | 6677 | 60 | 0.03308 |
| 3.800 | 6677 | 60 | 0.03308 |
| phosphonite | 3.459 | 6677 | 105 | 0.03316 |
| 3.600 | 6677 | 105 | 0.03316 |
| 3.800 | 6677 | 105 | 0.03316 |
| phosphinite | Compound\_1 | 3.459 | 6666 | 205 | 0.03336 |
| 3.600 | 6666 | 205 | 0.03336 |
| 3.800 | 6666 | 205 | 0.03336 |
| phosphonite | Compound\_3 | 3.459 | 6666 | 168 | 0.03359 |
| 3.600 | 6666 | 168 | 0.03359 |
| 3.800 | 6666 | 168 | 0.03359 |
| phosphonamidite | 3.459 | 6677 | 126 | 0.03361 |
| 3.600 | 6677 | 126 | 0.03361 |
| 3.800 | 6677 | 126 | 0.03361 |
| phosphate | 3.459 | 6677 | 7 | 0.03395 |
| 3.600 | 6677 | 7 | 0.03395 |
| 3.800 | 6677 | 7 | 0.03395 |
| 3.459 | 6666 | 14 | 0.03401 |
| 3.600 | 6666 | 14 | 0.03401 |
| 3.800 | 6666 | 14 | 0.03401 |
| phosphonamidite | 3.459 | 6666 | 188 | 0.03402 |
| 3.600 | 6666 | 188 | 0.03402 |
| 3.800 | 6666 | 188 | 0.03402 |
| phosphinite | Compound\_2 | 3.459 | 6677 | 148 | 0.03419 |
| 3.600 | 6677 | 148 | 0.03419 |
| 3.800 | 6677 | 148 | 0.03419 |
| 3.459 | 6666 | 207 | 0.03450 |
| 3.600 | 6666 | 207 | 0.03450 |
| 3.800 | 6666 | 207 | 0.03450 |
| phosphonamidate | Compound\_1 | 3.459 | 6677 | 18 | 0.03452 |
| 3.600 | 6677 | 18 | 0.03452 |
| 3.800 | 6677 | 18 | 0.03452 |
| 3.459 | 6666 | 21 | 0.03456 |
| 3.600 | 6666 | 21 | 0.03456 |
| 3.800 | 6666 | 21 | 0.03456 |
| phosphonite | Compound\_2 | 3.459 | 6677 | 126 | 0.03478 |
| 3.600 | 6677 | 126 | 0.03478 |
| 3.800 | 6677 | 126 | 0.03478 |
| phosphine | 3.459 | 6677 | 172 | 0.03488 |
| 3.600 | 6677 | 172 | 0.03488 |
| 3.800 | 6677 | 172 | 0.03488 |
| 3.459 | 6666 | 238 | 0.03507 |
| 3.600 | 6666 | 238 | 0.03507 |
| 3.800 | 6666 | 238 | 0.03507 |
| phosphonite | 3.459 | 6666 | 186 | 0.03518 |
| 3.600 | 6666 | 186 | 0.03518 |
| 3.800 | 6666 | 186 | 0.03518 |
| phosphinamidate | Compound\_3 | 3.459 | 6666 | 32 | 0.03524 |
| 3.600 | 6666 | 32 | 0.03524 |
| 3.800 | 6666 | 32 | 0.03524 |
| 3.459 | 6677 | 42 | 0.03528 |
| 3.600 | 6677 | 42 | 0.03528 |
| 3.800 | 6677 | 42 | 0.03528 |
| phosphite | 3.459 | 6677 | 133 | 0.03543 |
| 3.600 | 6677 | 133 | 0.03543 |
| 3.800 | 6677 | 133 | 0.03543 |
| phosphine | Compound\_1 | 3.459 | 6677 | 180 | 0.03554 |
| 3.600 | 6677 | 180 | 0.03554 |
| 3.800 | 6677 | 180 | 0.03554 |
| phosphinamidate | 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 | 244 | 0.03575 |
| 3.600 | 6666 | 244 | 0.03575 |
| 3.800 | 6666 | 244 | 0.03575 |
| phosphinamidate | 3.459 | 6677 | 51 | 0.03577 |
| 3.600 | 6677 | 51 | 0.03577 |
| 3.800 | 6677 | 51 | 0.03577 |
| phosphorodiamidite | Compound\_2 | 3.459 | 6677 | 104 | 0.03584 |
| 3.600 | 6677 | 1 | 0.03584 |
| 3.800 | 6677 | 104 | 0.03584 |
| phosphinate | Compound\_1 | 3.459 | 6677 | 42 | 0.03586 |
| 3.600 | 6677 | 42 | 0.03586 |
| 3.800 | 6677 | 42 | 0.03586 |
| phosphite | Compound\_3 | 3.459 | 6666 | 193 | 0.03594 |
| 3.600 | 6666 | 193 | 0.03594 |
| 3.800 | 6666 | 193 | 0.03594 |
| phosphorodiamidite | Compound\_2 | 3.459 | 6666 | 172 | 0.03624 |
| 3.800 | 6666 | 172 | 0.03624 |
| phosphinamidite | Compound\_1 | 3.459 | 6677 | 184 | 0.03628 |
| 3.600 | 6677 | 184 | 0.03628 |
| 3.800 | 6677 | 184 | 0.03628 |
| phosphineoxide | 3.459 | 6666 | 32 | 0.03631 |
| 3.600 | 6666 | 32 | 0.03631 |
| 3.800 | 6666 | 32 | 0.03631 |
| 3.459 | 6677 | 43 | 0.03634 |
| 3.600 | 6677 | 43 | 0.03634 |
| 3.800 | 6677 | 43 | 0.03634 |
| phosphinamidite | 3.459 | 6666 | 238 | 0.03647 |
| 3.600 | 6666 | 238 | 0.03647 |
| 3.800 | 6666 | 238 | 0.03647 |
| phosphoroamidate | 3.459 | 6666 | 16 | 0.03654 |
| 3.600 | 6666 | 16 | 0.03654 |
| 3.800 | 6666 | 16 | 0.03654 |
| 3.459 | 6677 | 23 | 0.03656 |
| 3.600 | 6677 | 23 | 0.03656 |
| 3.800 | 6677 | 23 | 0.03656 |
| phosphondiamidate | 3.459 | 6666 | 47 | 0.03666 |
| 3.600 | 6666 | 47 | 0.03666 |
| 3.800 | 6666 | 47 | 0.03666 |
| 3.459 | 6677 | 68 | 0.03671 |
| 3.600 | 6677 | 68 | 0.03671 |
| 3.800 | 6677 | 68 | 0.03671 |
| phosphorodiamidate | Compound\_2 | 3.459 | 6677 | 23 | 0.03673 |
| 3.600 | 6677 | 23 | 0.03673 |
| 3.800 | 6677 | 23 | 0.03673 |
| 3.459 | 6666 | 26 | 0.03675 |
| 3.600 | 6666 | 26 | 0.03675 |
| 3.800 | 6666 | 26 | 0.03675 |
| phosphineoxide | Compound\_3 | 3.459 | 6666 | 64 | 0.03695 |
| 3.600 | 6666 | 64 | 0.03695 |
| 3.800 | 6666 | 64 | 0.03695 |
| 3.459 | 6677 | 108 | 0.03706 |
| 3.600 | 6677 | 108 | 0.03706 |
| 3.800 | 6677 | 108 | 0.03706 |
| phosphonamidate | 3.459 | 6677 | 15 | 0.03728 |
| 3.600 | 6677 | 15 | 0.03728 |
| 3.800 | 6677 | 15 | 0.03728 |
| phosphondiamidate | Compound\_2 | 3.600 | 6666 | 24 | 0.03732 |
| 3.800 | 6666 | 24 | 0.03732 |
| 3.459 | 6666 | 24 | 0.03733 |
| 3.459 | 6677 | 24 | 0.03733 |
| 3.600 | 6677 | 25 | 0.03733 |
| 3.800 | 6677 | 25 | 0.03733 |
| phosphonamidate | Compound\_3 | 3.459 | 6666 | 25 | 0.03734 |
| 3.600 | 6666 | 25 | 0.03734 |
| 3.800 | 6666 | 25 | 0.03734 |
| phosphorodiamidate | 3.459 | 6677 | 30 | 0.03740 |
| 3.600 | 6677 | 30 | 0.03740 |
| 3.800 | 6677 | 30 | 0.03740 |
| 3.459 | 6666 | 34 | 0.03742 |
| 3.600 | 6666 | 34 | 0.03742 |
| 3.800 | 6666 | 34 | 0.03742 |
| phosphonamidite | Compound\_1 | 3.459 | 6677 | 124 | 0.03773 |
| 3.600 | 6677 | 124 | 0.03773 |
| 3.800 | 6677 | 124 | 0.03773 |
| phosphoamidite | Compound\_3 | 3.459 | 6677 | 100 | 0.03793 |
| 3.600 | 6677 | 100 | 0.03793 |
| 3.800 | 6677 | 100 | 0.03793 |
| phosphonamidite | Compound\_1 | 3.459 | 6666 | 192 | 0.03810 |
| 3.600 | 6666 | 192 | 0.03810 |
| 3.800 | 6666 | 192 | 0.03810 |
| phosphate | Compound\_2 | 3.459 | 6677 | 3 | 0.03810 |
| 3.600 | 6677 | 3 | 0.03810 |
| 3.800 | 6677 | 3 | 0.03810 |
| 3.459 | 6666 | 7 | 0.03816 |
| 3.600 | 6666 | 7 | 0.03816 |
| 3.800 | 6666 | 7 | 0.03816 |
| phosphoamidite | Compound\_3 | 3.459 | 6666 | 167 | 0.03826 |
| 3.600 | 6666 | 167 | 0.03826 |
| 3.800 | 6666 | 167 | 0.03826 |
| phosphite | Compound\_1 | 3.459 | 6677 | 85 | 0.03829 |
| 3.600 | 6677 | 85 | 0.03829 |
| 3.800 | 6677 | 85 | 0.03829 |
| phosphonodiamidite | Compound\_3 | 3.459 | 6677 | 148 | 0.03836 |
| 3.600 | 6677 | 148 | 0.03836 |
| 3.800 | 6677 | 148 | 0.03836 |
| 3.459 | 6666 | 206 | 0.03855 |
| 3.600 | 6666 | 206 | 0.03855 |
| 3.800 | 6666 | 206 | 0.03855 |
| phosphite | Compound\_1 | 3.459 | 6666 | 159 | 0.03870 |
| 3.600 | 6666 | 159 | 0.03870 |
| 3.800 | 6666 | 159 | 0.03870 |
| phosphinamidite | Compound\_3 | 3.459 | 6677 | 164 | 0.03876 |
| 3.600 | 6677 | 164 | 0.03876 |
| 3.800 | 6677 | 164 | 0.03876 |
| phosphorotriamidite | Compound\_1 | 3.459 | 6677 | 151 | 0.03877 |
| 3.600 | 6677 | 151 | 0.03877 |
| 3.800 | 6677 | 151 | 0.03877 |
| phosphinamidite | Compound\_3 | 3.459 | 6666 | 233 | 0.03901 |
| 3.600 | 6666 | 233 | 0.03901 |
| 3.800 | 6666 | 233 | 0.03901 |
| phosphite | Compound\_2 | 3.459 | 6677 | 94 | 0.03901 |
| 3.600 | 6677 | 94 | 0.03901 |
| 3.800 | 6677 | 94 | 0.03901 |
| phosphorotriamidite | Compound\_1 | 3.459 | 6666 | 213 | 0.03925 |
| 3.600 | 6666 | 213 | 0.03925 |
| 3.800 | 6666 | 213 | 0.03925 |
| phosphoamidite | Compound\_2 | 3.459 | 6677 | 130 | 0.03929 |
| 3.600 | 6677 | 130 | 0.03929 |
| 3.800 | 6677 | 130 | 0.03929 |
| phosphite | 3.459 | 6666 | 163 | 0.03942 |
| 3.600 | 6666 | 163 | 0.03942 |
| 3.800 | 6666 | 163 | 0.03942 |
| phosphoamidite | 3.459 | 6666 | 189 | 0.03967 |
| 3.600 | 6666 | 189 | 0.03967 |
| 3.800 | 6666 | 189 | 0.03967 |
| phosphorotriamidate | Compound\_3 | 3.459 | 6677 | 34 | 0.03972 |
| 3.600 | 6677 | 34 | 0.03972 |
| 3.800 | 6677 | 34 | 0.03972 |
| 3.459 | 6666 | 40 | 0.03974 |
| 3.600 | 6666 | 40 | 0.03974 |
| 3.800 | 6666 | 40 | 0.03974 |
| phosphonite | Compound\_1 | 3.459 | 6677 | 115 | 0.04005 |
| 3.600 | 6677 | 115 | 0.04005 |
| 3.800 | 6677 | 115 | 0.04005 |
| phosphinite | Compound\_3 | 3.459 | 6677 | 163 | 0.04008 |
| 3.600 | 6677 | 163 | 0.04008 |
| 3.800 | 6677 | 163 | 0.04008 |
| phosphine | 3.459 | 6677 | 209 | 0.04009 |
| 3.600 | 6677 | 209 | 0.04009 |
| 3.800 | 6677 | 209 | 0.04009 |
| phosphoamidite | Compound\_1 | 3.459 | 6677 | 106 | 0.04010 |
| 3.600 | 6677 | 106 | 0.04010 |
| 3.800 | 6677 | 106 | 0.04010 |
| phosphonamidite | Compound\_2 | 3.459 | 6677 | 138 | 0.04032 |
| 3.600 | 6677 | 138 | 0.04032 |
| 3.800 | 6677 | 138 | 0.04032 |
| phosphinite | Compound\_3 | 3.459 | 6666 | 232 | 0.04037 |
| 3.600 | 6666 | 232 | 0.04037 |
| 3.800 | 6666 | 232 | 0.04037 |
| phosphonite | Compound\_1 | 3.459 | 6666 | 180 | 0.04037 |
| 3.600 | 6666 | 180 | 0.04037 |
| 3.800 | 6666 | 180 | 0.04037 |
| phosphine | Compound\_3 | 3.459 | 6666 | 261 | 0.04038 |
| 3.600 | 6666 | 261 | 0.04038 |
| 3.800 | 6666 | 261 | 0.04038 |
| phosphoamidite | Compound\_1 | 3.459 | 6666 | 174 | 0.04046 |
| 3.600 | 6666 | 174 | 0.04046 |
| 3.800 | 6666 | 174 | 0.04046 |
| phosphonamidite | Compound\_2 | 3.459 | 6666 | 210 | 0.04060 |
| 3.600 | 6666 | 210 | 0.04060 |
| 3.800 | 6666 | 210 | 0.04060 |
| phosphoroamidate | 3.459 | 6677 | 9 | 0.04103 |
| 3.600 | 6677 | 9 | 0.04103 |
| 3.800 | 6677 | 9 | 0.04103 |
| 3.459 | 6666 | 12 | 0.04104 |
| 3.600 | 6666 | 12 | 0.04104 |
| 3.800 | 6666 | 12 | 0.04104 |
| phosphorodiamidite | 3.600 | 6666 | 12 | 0.04104 |
| Compound\_3 | 3.459 | 6677 | 135 | 0.04133 |
| 3.600 | 6677 | 135 | 0.04133 |
| 3.800 | 6677 | 135 | 0.04133 |
| 3.459 | 6666 | 190 | 0.04168 |
| 3.600 | 6666 | 190 | 0.04168 |
| 3.800 | 6666 | 190 | 0.04168 |
| phosphonodiamidite | Compound\_2 | 3.459 | 6677 | 143 | 0.04213 |
| 3.600 | 6677 | 143 | 0.04213 |
| 3.800 | 6677 | 143 | 0.04213 |
| 3.459 | 6666 | 216 | 0.04245 |
| 3.600 | 6666 | 216 | 0.04245 |
| 3.800 | 6666 | 216 | 0.04245 |
| phosphinate | Compound\_3 | 3.459 | 6666 | 19 | 0.04252 |
| 3.600 | 6666 | 19 | 0.04252 |
| 3.800 | 6666 | 19 | 0.04252 |
| 3.459 | 6677 | 27 | 0.04256 |
| 3.600 | 6677 | 27 | 0.04256 |
| 3.800 | 6677 | 27 | 0.04256 |
| phosphorotriamidate | Compound\_2 | 3.459 | 6677 | 29 | 0.04271 |
| 3.600 | 6677 | 29 | 0.04271 |
| 3.800 | 6677 | 29 | 0.04271 |
| 3.459 | 6666 | 36 | 0.04273 |
| 3.600 | 6666 | 36 | 0.04273 |
| 3.800 | 6666 | 36 | 0.04273 |
| phosphineoxide | 3.459 | 6666 | 128 | 0.04301 |
| 3.600 | 6666 | 128 | 0.04301 |
| 3.800 | 6666 | 128 | 0.04301 |
| 3.459 | 6677 | 136 | 0.04302 |
| 3.600 | 6677 | 136 | 0.04302 |
| 3.800 | 6677 | 136 | 0.04302 |
| phosphondiamidate | Compound\_3 | 3.459 | 6666 | 29 | 0.04321 |
| 3.600 | 6666 | 29 | 0.04321 |
| 3.800 | 6666 | 29 | 0.04321 |
| phosphonamidate | Compound\_2 | 3.459 | 6666 | 30 | 0.04324 |
| 3.600 | 6666 | 30 | 0.04324 |
| 3.800 | 6666 | 30 | 0.04324 |
| phosphondiamidate | Compound\_3 | 3.459 | 6677 | 44 | 0.04327 |
| 3.600 | 6677 | 44 | 0.04327 |
| 3.800 | 6677 | 44 | 0.04327 |
| phosphonamidate | Compound\_2 | 3.459 | 6677 | 39 | 0.04330 |
| 3.600 | 6677 | 39 | 0.04330 |
| 3.800 | 6677 | 39 | 0.04330 |
| phosphorotriamidite | Compound\_3 | 3.459 | 6677 | 174 | 0.04343 |
| 3.600 | 6677 | 174 | 0.04343 |
| 3.800 | 6677 | 174 | 0.04343 |
| 3.459 | 6666 | 228 | 0.04366 |
| 3.600 | 6666 | 228 | 0.04366 |
| 3.800 | 6666 | 228 | 0.04366 |
| phosphorotriamidate | Compound\_1 | 3.600 | 6677 | 76 | 0.04481 |
| 3.800 | 6677 | 47 | 0.04481 |
| 3.459 | 6677 | 52 | 0.04483 |
| phosphinamidate | Compound\_2 | 3.459 | 6677 | 42 | 0.04494 |
| 3.600 | 6677 | 42 | 0.04494 |
| 3.800 | 6677 | 42 | 0.04494 |
| 3.459 | 6666 | 54 | 0.04500 |
| 3.600 | 6666 | 54 | 0.04500 |
| 3.800 | 6666 | 54 | 0.04500 |
| phosphorotriamidate | Compound\_1 | 3.600 | 6666 | 141 | 0.04503 |
| 3.800 | 6666 | 162 | 0.04517 |
| 3.459 | 6666 | 164 | 0.04518 |
| phosphorodiamidite | 3.459 | 6677 | 129 | 0.04614 |
| 3.600 | 6677 | 129 | 0.04614 |
| 3.800 | 6677 | 129 | 0.04614 |
| phosphinamidite | Compound\_2 | 3.459 | 6677 | 150 | 0.04635 |
| 3.600 | 6677 | 150 | 0.04635 |
| 3.800 | 6677 | 150 | 0.04635 |
| phosphorodiamidite | Compound\_1 | 3.459 | 6666 | 191 | 0.04647 |
| 3.600 | 6666 | 191 | 0.04647 |
| 3.800 | 6666 | 191 | 0.04647 |
| phosphinamidite | Compound\_2 | 3.459 | 6666 | 192 | 0.04652 |
| 3.600 | 6666 | 193 | 0.04652 |
| 3.800 | 6666 | 193 | 0.04652 |
| phosphorotriamidite | 3.459 | 6677 | 153 | 0.04693 |
| 3.600 | 6677 | 157 | 0.04694 |
| 3.800 | 6677 | 157 | 0.04694 |
| 3.459 | 6666 | 218 | 0.04718 |
| 3.600 | 6666 | 218 | 0.04718 |
| 3.800 | 6666 | 218 | 0.04718 |
| phosphonodiamidite | Compound\_1 | 3.459 | 6677 | 154 | 0.04757 |
| 3.600 | 6677 | 154 | 0.04757 |
| 3.800 | 6677 | 154 | 0.04757 |
| 3.459 | 6666 | 212 | 0.04786 |
| 3.600 | 6666 | 212 | 0.04786 |
| 3.800 | 6666 | 212 | 0.04786 |