Summary Tables

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# Tables for Top 5 and Bottom 5.

Tables are filtered for Atom as the phosphate only.

## Top 5

**Table** : Top 5 scoring RMSD MAP

| **Chemical Group** | **Compound** | ***n*(l)** | **RMSD\_MAP** | **Rank** |
| --- | --- | --- | --- | --- |
| phosphate | 1 | 4555 | 0.02795 | 1 |
| 5555 | 0.02795 | 1 |
| 5666 | 0.02801 | 3 |
| 6666 | 0.02802 | 4 |
| 4455 | 0.02807 | 5 |
| 6677 | 0.02821 | 18 |
| 2 | 5566 | 0.03807 | 1 |
| 6566 | 0.03809 | 2 |
| 6677 | 0.03810 | 3 |
| 4566 | 0.03811 | 4 |
| 4455 | 0.03812 | 5 |
| 6666 | 0.03816 | 7 |
| 3 | 5566 | 0.03388 | 1 |
| 4455 | 0.03390 | 2 |
| 5567 | 0.03392 | 3 |
| 4555 | 0.03393 | 4 |
| 4566 | 0.03393 | 4 |
| 5666 | 0.03393 | 4 |
| 6677 | 0.03395 | 7 |
| 6666 | 0.03401 | 14 |
| phosphinamidate | 1 | 5556 | 0.03550 | 1 |
| 4456 | 0.03552 | 2 |
| 4556 | 0.03552 | 2 |
| 4445 | 0.03554 | 4 |
| 5456 | 0.03554 | 4 |
| 6666 | 0.03566 | 26 |
| 6677 | 0.03577 | 51 |
| 2 | 4556 | 0.04467 | 1 |
| 3445 | 0.04470 | 2 |
| 3556 | 0.04472 | 3 |
| 4555 | 0.04472 | 3 |
| 5667 | 0.04474 | 5 |
| 6677 | 0.04494 | 42 |
| 6666 | 0.04500 | 54 |
| 3 | 4556 | 0.03502 | 1 |
| 5556 | 0.03503 | 2 |
| 4456 | 0.03506 | 3 |
| 3445 | 0.03507 | 4 |
| 4445 | 0.03507 | 4 |
| 6666 | 0.03524 | 32 |
| 6677 | 0.03528 | 42 |
| phosphinamidite | 1 | 2256 | 0.03540 | 1 |
| 2356 | 0.03540 | 1 |
| 2367 | 0.03543 | 3 |
| 2357 | 0.03545 | 4 |
| 2467 | 0.03545 | 4 |
| 6677 | 0.03628 | 184 |
| 6666 | 0.03647 | 238 |
| 2 | 2456 | 0.04577 | 1 |
| 2356 | 0.04578 | 2 |
| 2467 | 0.04578 | 2 |
| 2567 | 0.04579 | 4 |
| 2355 | 0.04581 | 5 |
| 2367 | 0.04581 | 5 |
| 2455 | 0.04581 | 5 |
| 2466 | 0.04581 | 5 |
| 6677 | 0.04635 | 150 |
| 6666 | 0.04652 | 192 |
| 3 | 2256 | 0.03794 | 1 |
| 2367 | 0.03794 | 1 |
| 2267 | 0.03795 | 3 |
| 2356 | 0.03796 | 4 |
| 2467 | 0.03797 | 5 |
| 6677 | 0.03876 | 164 |
| 6666 | 0.03901 | 233 |
| phosphinate | 1 | 5555 | 0.03564 | 1 |
| 5556 | 0.03564 | 1 |
| 4556 | 0.03565 | 3 |
| 4555 | 0.03566 | 4 |
| 6666 | 0.03569 | 5 |
| 6667 | 0.03569 | 5 |
| 6677 | 0.03586 | 42 |
| 2 | 4556 | 0.03271 | 1 |
| 3556 | 0.03277 | 2 |
| 4456 | 0.03277 | 2 |
| 3445 | 0.03278 | 4 |
| 5556 | 0.03278 | 4 |
| 6666 | 0.03297 | 35 |
| 6677 | 0.03305 | 51 |
| 3 | 4556 | 0.04244 | 1 |
| 4455 | 0.04245 | 2 |
| 4456 | 0.04245 | 2 |
| 4555 | 0.04245 | 2 |
| 5556 | 0.04247 | 5 |
| 5566 | 0.04247 | 5 |
| 5567 | 0.04247 | 5 |
| 5667 | 0.04247 | 5 |
| 6666 | 0.04252 | 19 |
| 6677 | 0.04256 | 27 |
| phosphine | 1 | 2356 | 0.03476 | 1 |
| 2467 | 0.03476 | 1 |
| 2367 | 0.03477 | 3 |
| 2256 | 0.03478 | 4 |
| 2357 | 0.03479 | 5 |
| 2468 | 0.03479 | 5 |
| 6677 | 0.03554 | 180 |
| 6666 | 0.03575 | 244 |
| 2 | 2356 | 0.03402 | 1 |
| 2367 | 0.03402 | 1 |
| 2467 | 0.03402 | 1 |
| 2256 | 0.03403 | 4 |
| 2267 | 0.03406 | 5 |
| 6677 | 0.03488 | 172 |
| 6666 | 0.03507 | 238 |
| 3 | 2367 | 0.03892 | 1 |
| 2467 | 0.03892 | 1 |
| 2468 | 0.03895 | 3 |
| 2368 | 0.03897 | 4 |
| 2267 | 0.03900 | 5 |
| 2356 | 0.03900 | 5 |
| 6677 | 0.04009 | 209 |
| 6666 | 0.04038 | 261 |
| phosphineoxide | 1 | 4456 | 0.03615 | 1 |
| 4556 | 0.03617 | 2 |
| 3345 | 0.03618 | 3 |
| 3445 | 0.03619 | 4 |
| 3456 | 0.03619 | 4 |
| 4455 | 0.03619 | 4 |
| 6666 | 0.03631 | 32 |
| 6677 | 0.03634 | 43 |
| 2 | 4445 | 0.04270 | 1 |
| 3445 | 0.04272 | 2 |
| 4345 | 0.04272 | 2 |
| 4456 | 0.04272 | 2 |
| 3345 | 0.04273 | 5 |
| 4556 | 0.04273 | 5 |
| 5456 | 0.04273 | 5 |
| 6666 | 0.04301 | 128 |
| 6677 | 0.04302 | 136 |
| 3 | 4445 | 0.03665 | 1 |
| 5556 | 0.03666 | 2 |
| 4556 | 0.03668 | 3 |
| 3445 | 0.03669 | 4 |
| 5445 | 0.03671 | 5 |
| 6666 | 0.03695 | 64 |
| 6677 | 0.03706 | 108 |
| phosphinite | 1 | 2356 | 0.03220 | 1 |
| 2467 | 0.03221 | 2 |
| 2456 | 0.03223 | 3 |
| 2367 | 0.03227 | 4 |
| 2567 | 0.03227 | 4 |
| 6677 | 0.03302 | 138 |
| 6666 | 0.03336 | 205 |
| 2 | 2467 | 0.03324 | 1 |
| 2367 | 0.03326 | 2 |
| 2567 | 0.03328 | 3 |
| 2356 | 0.03329 | 4 |
| 2267 | 0.03332 | 5 |
| 2456 | 0.03332 | 5 |
| 2466 | 0.03332 | 5 |
| 6677 | 0.03419 | 148 |
| 6666 | 0.03450 | 207 |
| 3 | 2356 | 0.03919 | 1 |
| 2467 | 0.03922 | 2 |
| 2456 | 0.03923 | 3 |
| 2367 | 0.03926 | 4 |
| 2256 | 0.03927 | 5 |
| 2357 | 0.03927 | 5 |
| 6677 | 0.04008 | 163 |
| 6666 | 0.04037 | 232 |
| phosphite | 1 | 2466 | 0.03736 | 1 |
| 2467 | 0.03740 | 2 |
| 2366 | 0.03743 | 3 |
| 2566 | 0.03745 | 4 |
| 2567 | 0.03746 | 5 |
| 6677 | 0.03829 | 85 |
| 6666 | 0.03870 | 159 |
| 2 | 2466 | 0.03824 | 1 |
| 2467 | 0.03827 | 2 |
| 2566 | 0.03828 | 3 |
| 2567 | 0.03829 | 4 |
| 2366 | 0.03834 | 5 |
| 6677 | 0.03901 | 94 |
| 6666 | 0.03942 | 163 |
| 3 | 2456 | 0.03461 | 1 |
| 3567 | 0.03462 | 2 |
| 2567 | 0.03465 | 3 |
| 2556 | 0.03467 | 4 |
| 2356 | 0.03468 | 5 |
| 2467 | 0.03468 | 5 |
| 3467 | 0.03468 | 5 |
| 3667 | 0.03468 | 5 |
| 6677 | 0.03543 | 133 |
| 6666 | 0.03594 | 193 |
| phosphoamidite | 1 | 2466 | 0.03932 | 1 |
| 2467 | 0.03932 | 1 |
| 2567 | 0.03937 | 3 |
| 2356 | 0.03940 | 4 |
| 2366 | 0.03940 | 4 |
| 2566 | 0.03940 | 4 |
| 6677 | 0.04010 | 106 |
| 6666 | 0.04046 | 174 |
| 2 | 2356 | 0.03855 | 1 |
| 2456 | 0.03855 | 1 |
| 2355 | 0.03856 | 3 |
| 2466 | 0.03857 | 4 |
| 2455 | 0.03858 | 5 |
| 2467 | 0.03858 | 5 |
| 6677 | 0.03929 | 130 |
| 6666 | 0.03967 | 189 |
| 3 | 2466 | 0.03717 | 1 |
| 2467 | 0.03720 | 2 |
| 2355 | 0.03725 | 3 |
| 2566 | 0.03725 | 3 |
| 2567 | 0.03725 | 3 |
| 6677 | 0.03793 | 100 |
| 6666 | 0.03826 | 167 |
| phosphonamidate | 1 | 4456 | 0.03439 | 1 |
| 5567 | 0.03439 | 1 |
| 4455 | 0.03441 | 3 |
| 5566 | 0.03442 | 4 |
| 4556 | 0.03445 | 5 |
| 4567 | 0.03445 | 5 |
| 6677 | 0.03452 | 18 |
| 6666 | 0.03456 | 21 |
| 2 | 5456 | 0.04307 | 1 |
| 4456 | 0.04308 | 2 |
| 4345 | 0.04312 | 3 |
| 5455 | 0.04312 | 3 |
| 5556 | 0.04312 | 3 |
| 6456 | 0.04312 | 3 |
| 6666 | 0.04324 | 30 |
| 6677 | 0.04330 | 39 |
| 3 | 4456 | 0.03715 | 1 |
| 5567 | 0.03715 | 1 |
| 4567 | 0.03717 | 3 |
| 5566 | 0.03718 | 4 |
| 4455 | 0.03719 | 5 |
| 6677 | 0.03728 | 15 |
| 6666 | 0.03734 | 25 |
| phosphonamidite | 1 | 2467 | 0.03685 | 1 |
| 2466 | 0.03688 | 2 |
| 2567 | 0.03690 | 3 |
| 2356 | 0.03693 | 4 |
| 2367 | 0.03694 | 5 |
| 2456 | 0.03694 | 5 |
| 6677 | 0.03773 | 124 |
| 6666 | 0.03810 | 192 |
| 2 | 2467 | 0.03947 | 1 |
| 2356 | 0.03948 | 2 |
| 2367 | 0.03949 | 3 |
| 2466 | 0.03950 | 4 |
| 2366 | 0.03951 | 5 |
| 6677 | 0.04032 | 138 |
| 6666 | 0.04060 | 210 |
| 3 | 2467 | 0.03262 | 1 |
| 2466 | 0.03263 | 2 |
| 2567 | 0.03267 | 3 |
| 2366 | 0.03269 | 4 |
| 2356 | 0.03270 | 5 |
| 2566 | 0.03270 | 5 |
| 6677 | 0.03361 | 126 |
| 6666 | 0.03402 | 188 |
| phosphonate | 1 | 5555 | 0.02976 | 1 |
| 5556 | 0.02978 | 2 |
| 4555 | 0.02979 | 3 |
| 6666 | 0.02979 | 3 |
| 6667 | 0.02980 | 5 |
| 6677 | 0.03000 | 34 |
| 2 | 5555 | 0.03060 | 1 |
| 4555 | 0.03063 | 2 |
| 5556 | 0.03065 | 3 |
| 4556 | 0.03067 | 4 |
| 5666 | 0.03067 | 4 |
| 6666 | 0.03067 | 4 |
| 6677 | 0.03088 | 33 |
| 3 | 4556 | 0.03271 | 1 |
| 4456 | 0.03274 | 2 |
| 3445 | 0.03276 | 3 |
| 3456 | 0.03276 | 3 |
| 3556 | 0.03276 | 3 |
| 6666 | 0.03302 | 42 |
| 6677 | 0.03308 | 60 |
| phosphondiamidate | 1 | 4556 | 0.03641 | 1 |
| 4456 | 0.03643 | 2 |
| 3456 | 0.03645 | 3 |
| 3556 | 0.03646 | 4 |
| 5556 | 0.03647 | 5 |
| 5567 | 0.03647 | 5 |
| 5667 | 0.03647 | 5 |
| 6666 | 0.03666 | 47 |
| 6677 | 0.03671 | 68 |
| 2 | 4556 | 0.03715 | 1 |
| 5556 | 0.03715 | 1 |
| 4456 | 0.03716 | 3 |
| 5567 | 0.03718 | 4 |
| 5456 | 0.03719 | 5 |
| 5667 | 0.03719 | 5 |
| 6666 | 0.03733 | 24 |
| 6677 | 0.03733 | 24 |
| 3 | 4456 | 0.04306 | 1 |
| 5556 | 0.04308 | 2 |
| 4556 | 0.04309 | 3 |
| 5456 | 0.04309 | 3 |
| 5567 | 0.04310 | 5 |
| 6666 | 0.04321 | 29 |
| 6677 | 0.04327 | 44 |
| phosphonite | 1 | 2467 | 0.03928 | 1 |
| 2466 | 0.03929 | 2 |
| 2567 | 0.03930 | 3 |
| 2566 | 0.03933 | 4 |
| 2456 | 0.03934 | 5 |
| 6677 | 0.04005 | 115 |
| 6666 | 0.04037 | 180 |
| 2 | 2456 | 0.03379 | 1 |
| 2467 | 0.03381 | 2 |
| 2567 | 0.03381 | 2 |
| 2356 | 0.03387 | 4 |
| 2466 | 0.03388 | 5 |
| 6677 | 0.03478 | 126 |
| 6666 | 0.03518 | 186 |
| 3 | 2466 | 0.03229 | 1 |
| 2566 | 0.03229 | 1 |
| 2567 | 0.03230 | 3 |
| 2455 | 0.03231 | 4 |
| 2456 | 0.03231 | 4 |
| 6677 | 0.03316 | 105 |
| 6666 | 0.03359 | 168 |
| phosphonodiamidite | 1 | 2356 | 0.04686 | 1 |
| 2367 | 0.04686 | 1 |
| 2467 | 0.04686 | 1 |
| 2256 | 0.04687 | 4 |
| 2267 | 0.04690 | 5 |
| 2366 | 0.04690 | 5 |
| 2456 | 0.04690 | 5 |
| 6677 | 0.04757 | 154 |
| 6666 | 0.04786 | 212 |
| 2 | 2367 | 0.04129 | 1 |
| 2467 | 0.04129 | 1 |
| 2366 | 0.04131 | 3 |
| 2356 | 0.04132 | 4 |
| 2466 | 0.04132 | 4 |
| 6677 | 0.04213 | 143 |
| 6666 | 0.04245 | 216 |
| 3 | 2467 | 0.03749 | 1 |
| 2567 | 0.03752 | 2 |
| 2356 | 0.03754 | 3 |
| 2456 | 0.03754 | 3 |
| 2466 | 0.03754 | 3 |
| 6677 | 0.03836 | 148 |
| 6666 | 0.03855 | 206 |
| phosphoroamidate | 1 | 4556 | 0.03643 | 1 |
| 4555 | 0.03645 | 2 |
| 5667 | 0.03645 | 2 |
| 4456 | 0.03646 | 4 |
| 5567 | 0.03646 | 4 |
| 6666 | 0.03654 | 16 |
| 6677 | 0.03656 | 23 |
| 2 | 5667 | 0.04096 | 1 |
| 5567 | 0.04097 | 2 |
| 5566 | 0.04099 | 3 |
| 5666 | 0.04099 | 3 |
| 4556 | 0.04100 | 5 |
| 6667 | 0.04100 | 5 |
| 6677 | 0.04103 | 9 |
| 6666 | 0.04104 | 12 |
| 3 | 5667 | 0.03130 | 1 |
| 4556 | 0.03132 | 2 |
| 5666 | 0.03132 | 2 |
| 4555 | 0.03133 | 4 |
| 5567 | 0.03134 | 5 |
| 6666 | 0.03144 | 15 |
| 6677 | 0.03144 | 15 |
| phosphorodiamidate | 1 | 4456 | 0.03214 | 1 |
| 4556 | 0.03215 | 2 |
| 4567 | 0.03215 | 2 |
| 3456 | 0.03216 | 4 |
| 5567 | 0.03216 | 4 |
| 6677 | 0.03241 | 34 |
| 6666 | 0.03244 | 42 |
| 2 | 4456 | 0.03658 | 1 |
| 5567 | 0.03658 | 1 |
| 4556 | 0.03659 | 3 |
| 4567 | 0.03662 | 4 |
| 5667 | 0.03662 | 4 |
| 6677 | 0.03673 | 23 |
| 6666 | 0.03675 | 26 |
| 3 | 4456 | 0.03718 | 1 |
| 5567 | 0.03721 | 2 |
| 3456 | 0.03723 | 3 |
| 4556 | 0.03723 | 3 |
| 4567 | 0.03723 | 3 |
| 6677 | 0.03740 | 30 |
| 6666 | 0.03742 | 34 |
| phosphorodiamidite | 1 | 2467 | 0.04538 | 1 |
| 2466 | 0.04540 | 2 |
| 2567 | 0.04542 | 3 |
| 2356 | 0.04545 | 4 |
| 2366 | 0.04545 | 4 |
| 2367 | 0.04545 | 4 |
| 2566 | 0.04545 | 4 |
| 6677 | 0.04614 | 129 |
| 6666 | 0.04647 | 191 |
| 2 | 2466 | 0.03501 | 1 |
| 2467 | 0.03503 | 2 |
| 2567 | 0.03504 | 3 |
| 2566 | 0.03507 | 4 |
| 2456 | 0.03508 | 5 |
| 6677 | 0.03584 | 104 |
| 6666 | 0.03624 | 172 |
| 3 | 2467 | 0.04049 | 1 |
| 2567 | 0.04049 | 1 |
| 2456 | 0.04051 | 3 |
| 2466 | 0.04052 | 4 |
| 2356 | 0.04054 | 5 |
| 6677 | 0.04133 | 135 |
| 6666 | 0.04168 | 190 |
| phosphorotriamidate | 1 | 4456 | 0.04457 | 1 |
| 4556 | 0.04457 | 1 |
| 5456 | 0.04460 | 3 |
| 4445 | 0.04461 | 4 |
| 3445 | 0.04462 | 5 |
| 3456 | 0.04462 | 5 |
| 5567 | 0.04462 | 5 |
| 6677 | 0.04483 | 52 |
| 6666 | 0.04518 | 164 |
| 2 | 4456 | 0.04254 | 1 |
| 5456 | 0.04256 | 2 |
| 5567 | 0.04256 | 2 |
| 6567 | 0.04258 | 4 |
| 3456 | 0.04260 | 5 |
| 4567 | 0.04260 | 5 |
| 6677 | 0.04271 | 29 |
| 6666 | 0.04273 | 36 |
| 3 | 4456 | 0.03951 | 1 |
| 5567 | 0.03954 | 2 |
| 3456 | 0.03955 | 3 |
| 4556 | 0.03956 | 4 |
| 4567 | 0.03956 | 4 |
| 6677 | 0.03972 | 34 |
| 6666 | 0.03974 | 40 |
| phosphorotriamidite | 1 | 2367 | 0.03765 | 1 |
| 2356 | 0.03767 | 2 |
| 2467 | 0.03767 | 2 |
| 2256 | 0.03768 | 4 |
| 2366 | 0.03768 | 4 |
| 6677 | 0.03877 | 151 |
| 6666 | 0.03925 | 213 |
| 2 | 2367 | 0.04619 | 1 |
| 2256 | 0.04620 | 2 |
| 2356 | 0.04620 | 2 |
| 2467 | 0.04621 | 4 |
| 2267 | 0.04622 | 5 |
| 6677 | 0.04693 | 153 |
| 6666 | 0.04718 | 218 |
| 3 | 2256 | 0.04260 | 1 |
| 2356 | 0.04260 | 1 |
| 2367 | 0.04262 | 3 |
| 2467 | 0.04264 | 4 |
| 2267 | 0.04265 | 5 |
| 2456 | 0.04265 | 5 |
| 6677 | 0.04343 | 174 |
| 6666 | 0.04366 | 228 |

## Bottom 5

**Table** : Bottom 5 scoring RMSD MAP

| **drug** | **compound** | **alphavalue** | **nl** | **RMSD\_MAP** |
| --- | --- | --- | --- | --- |
| phosphate | Compound\_1 | 3.459 | 2248 | 0.03120 |
| 4248 | 0.03133 |
| 6247 | 0.03134 |
| 6258 | 0.03137 |
| 5248 | 0.03164 |
| 6248 | 0.03198 |
| Compound\_2 | 3648 | 0.04079 |
| 5648 | 0.04079 |
| 5248 | 0.04088 |
| 2648 | 0.04093 |
| 6648 | 0.04093 |
| 6248 | 0.04103 |
| Compound\_3 | 2248 | 0.03663 |
| 5648 | 0.03663 |
| 5248 | 0.03685 |
| 2648 | 0.03686 |
| 6648 | 0.03689 |
| 6248 | 0.03715 |
| phosphinamidate | Compound\_1 | 5248 | 0.03714 |
| 6548 | 0.03715 |
| 5648 | 0.03719 |
| 2648 | 0.03722 |
| 6248 | 0.03724 |
| 6648 | 0.03738 |
| Compound\_2 | 5265 | 0.04644 |
| 4248 | 0.04650 |
| 6265 | 0.04653 |
| 5248 | 0.04663 |
| 6648 | 0.04663 |
| 6248 | 0.04671 |
| Compound\_3 | 6548 | 0.03671 |
| 2648 | 0.03676 |
| 5648 | 0.03676 |
| 5248 | 0.03680 |
| 6248 | 0.03692 |
| 6648 | 0.03699 |
| phosphinamidite | Compound\_1 | 6348 | 0.03698 |
| 6647 | 0.03700 |
| 6448 | 0.03705 |
| 5648 | 0.03708 |
| 6548 | 0.03715 |
| 6648 | 0.03724 |
| Compound\_2 | 6647 | 0.04711 |
| 6448 | 0.04712 |
| 6248 | 0.04713 |
| 6548 | 0.04719 |
| 5648 | 0.04720 |
| 6648 | 0.04730 |
| Compound\_3 | 5647 | 0.03956 |
| 6448 | 0.03962 |
| 5548 | 0.03966 |
| 6548 | 0.03974 |
| 5648 | 0.03976 |
| 6648 | 0.03983 |
| phosphinate | Compound\_1 | 4248 | 0.03739 |
| 3248 | 0.03741 |
| 2648 | 0.03747 |
| 5248 | 0.03748 |
| 2248 | 0.03755 |
| 6248 | 0.03765 |
| Compound\_2 | 2265 | 0.03492 |
| 2248 | 0.03493 |
| 4248 | 0.03493 |
| 6648 | 0.03500 |
| 5248 | 0.03509 |
| 6248 | 0.03525 |
| Compound\_3 | 5648 | 0.04413 |
| 2248 | 0.04414 |
| 2648 | 0.04421 |
| 5248 | 0.04425 |
| 6648 | 0.04430 |
| 6248 | 0.04439 |
| phosphine | Compound\_1 | 5548 | 0.03619 |
| 6448 | 0.03619 |
| 6647 | 0.03620 |
| 5648 | 0.03631 |
| 6548 | 0.03631 |
| 6648 | 0.03642 |
| Compound\_2 | 6448 | 0.03559 |
| 6647 | 0.03560 |
| 5548 | 0.03562 |
| 6548 | 0.03572 |
| 5648 | 0.03574 |
| 6648 | 0.03584 |
| Compound\_3 | 5646 | 0.04078 |
| 5548 | 0.04083 |
| 6548 | 0.04088 |
| 5647 | 0.04093 |
| 5648 | 0.04102 |
| 6648 | 0.04112 |
| phosphineoxide | Compound\_1 | 2648 | 0.03738 |
| 6548 | 0.03738 |
| 5648 | 0.03743 |
| 6647 | 0.03743 |
| 6248 | 0.03747 |
| 6648 | 0.03767 |
| Compound\_2 | 2248 | 0.04358 |
| 5648 | 0.04358 |
| 6248 | 0.04360 |
| 3648 | 0.04361 |
| 2648 | 0.04369 |
| 6648 | 0.04369 |
| Compound\_3 | 4248 | 0.03797 |
| 2648 | 0.03800 |
| 2248 | 0.03801 |
| 5248 | 0.03803 |
| 6648 | 0.03803 |
| 6248 | 0.03808 |
| phosphinite | Compound\_1 | 6248 | 0.03423 |
| 6448 | 0.03423 |
| 6647 | 0.03434 |
| 5648 | 0.03437 |
| 6548 | 0.03439 |
| 6648 | 0.03458 |
| Compound\_2 | 5648 | 0.03554 |
| 6348 | 0.03557 |
| 6448 | 0.03559 |
| 6248 | 0.03561 |
| 6548 | 0.03569 |
| 6648 | 0.03582 |
| Compound\_3 | 5647 | 0.04095 |
| 6448 | 0.04097 |
| 6647 | 0.04111 |
| 5648 | 0.04113 |
| 6548 | 0.04114 |
| 6648 | 0.04133 |
| phosphite | Compound\_1 | 5548 | 0.04045 |
| 6647 | 0.04046 |
| 4648 | 0.04061 |
| 6548 | 0.04066 |
| 5648 | 0.04080 |
| 6648 | 0.04095 |
| Compound\_2 | 6647 | 0.04094 |
| 6448 | 0.04096 |
| 5648 | 0.04106 |
| 6248 | 0.04106 |
| 6548 | 0.04111 |
| 6648 | 0.04133 |
| Compound\_3 | 6247 | 0.03740 |
| 6448 | 0.03752 |
| 6548 | 0.03752 |
| 6648 | 0.03759 |
| 6348 | 0.03762 |
| 6248 | 0.03778 |
| phosphoamidite | Compound\_1 | 6448 | 0.04170 |
| 6647 | 0.04179 |
| 6248 | 0.04181 |
| 6548 | 0.04188 |
| 5648 | 0.04192 |
| 6648 | 0.04212 |
| Compound\_2 | 6647 | 0.04101 |
| 6348 | 0.04106 |
| 6448 | 0.04107 |
| 6248 | 0.04114 |
| 6548 | 0.04118 |
| 6648 | 0.04134 |
| Compound\_3 | 5548 | 0.03960 |
| 6647 | 0.03963 |
| 6248 | 0.03965 |
| 6548 | 0.03977 |
| 5648 | 0.03983 |
| 6648 | 0.04001 |
| phosphonamidate | Compound\_1 | 5648 | 0.03680 |
| 3648 | 0.03682 |
| 5248 | 0.03692 |
| 6648 | 0.03705 |
| 2648 | 0.03707 |
| 6248 | 0.03721 |
| Compound\_2 | 4648 | 0.04468 |
| 3648 | 0.04472 |
| 5648 | 0.04472 |
| 6248 | 0.04474 |
| 2648 | 0.04481 |
| 6648 | 0.04485 |
| Compound\_3 | 3648 | 0.03947 |
| 5248 | 0.03954 |
| 5648 | 0.03957 |
| 2648 | 0.03961 |
| 6248 | 0.03970 |
| 6648 | 0.03977 |
| phosphonamidite | Compound\_1 | 6448 | 0.03916 |
| 6248 | 0.03922 |
| 6647 | 0.03926 |
| 5648 | 0.03932 |
| 6548 | 0.03933 |
| 6648 | 0.03955 |
| Compound\_2 | 5647 | 0.04145 |
| 5548 | 0.04149 |
| 6647 | 0.04153 |
| 6548 | 0.04161 |
| 5648 | 0.04168 |
| 6648 | 0.04181 |
| Compound\_3 | 6248 | 0.03527 |
| 6448 | 0.03528 |
| 6647 | 0.03534 |
| 5648 | 0.03538 |
| 6548 | 0.03545 |
| 6648 | 0.03567 |
| phosphonate | Compound\_1 | 2648 | 0.03232 |
| 4248 | 0.03245 |
| 3248 | 0.03247 |
| 5248 | 0.03253 |
| 2248 | 0.03256 |
| 6248 | 0.03264 |
| Compound\_2 | 6348 | 0.03295 |
| 2248 | 0.03302 |
| 4248 | 0.03302 |
| 6247 | 0.03304 |
| 5248 | 0.03327 |
| 6248 | 0.03357 |
| Compound\_3 | 5648 | 0.03491 |
| 2648 | 0.03492 |
| 6348 | 0.03493 |
| 5248 | 0.03509 |
| 6648 | 0.03513 |
| 6248 | 0.03527 |
| phosphondiamidate | Compound\_1 | 5648 | 0.03831 |
| 6548 | 0.03835 |
| 6348 | 0.03837 |
| 5248 | 0.03841 |
| 6648 | 0.03852 |
| 6248 | 0.03858 |
| Compound\_2 | 6348 | 0.03891 |
| 6548 | 0.03894 |
| 5248 | 0.03896 |
| 2648 | 0.03898 |
| 6648 | 0.03914 |
| 6248 | 0.03916 |
| Compound\_3 | 3648 | 0.04458 |
| 5248 | 0.04458 |
| 5648 | 0.04460 |
| 2648 | 0.04472 |
| 6248 | 0.04473 |
| 6648 | 0.04478 |
| phosphonite | Compound\_1 | 6647 | 0.04151 |
| 5248 | 0.04152 |
| 5648 | 0.04158 |
| 6248 | 0.04160 |
| 6548 | 0.04163 |
| 6648 | 0.04183 |
| Compound\_2 | 5248 | 0.03637 |
| 6647 | 0.03648 |
| 6548 | 0.03651 |
| 5648 | 0.03653 |
| 6248 | 0.03653 |
| 6648 | 0.03683 |
| Compound\_3 | 5648 | 0.03523 |
| 6647 | 0.03523 |
| 5248 | 0.03527 |
| 6548 | 0.03530 |
| 6248 | 0.03544 |
| 6648 | 0.03559 |
| phosphonodiamidite | Compound\_1 | 6348 | 0.04856 |
| 6647 | 0.04859 |
| 6448 | 0.04862 |
| 5648 | 0.04864 |
| 6548 | 0.04872 |
| 6648 | 0.04882 |
| Compound\_2 | 5647 | 0.04324 |
| 6448 | 0.04328 |
| 5648 | 0.04341 |
| 6647 | 0.04341 |
| 6548 | 0.04345 |
| 6648 | 0.04363 |
| Compound\_3 | 5647 | 0.03932 |
| 4648 | 0.03934 |
| 5548 | 0.03939 |
| 6548 | 0.03941 |
| 5648 | 0.03958 |
| 6648 | 0.03960 |
| phosphoroamidate | Compound\_1 | 4248 | 0.03868 |
| 2248 | 0.03875 |
| 2648 | 0.03875 |
| 5248 | 0.03886 |
| 6648 | 0.03886 |
| 6248 | 0.03909 |
| Compound\_2 | 5648 | 0.04305 |
| 2248 | 0.04313 |
| 5248 | 0.04317 |
| 6648 | 0.04323 |
| 2648 | 0.04325 |
| 6248 | 0.04335 |
| Compound\_3 | 6348 | 0.03422 |
| 2248 | 0.03423 |
| 2648 | 0.03425 |
| 5248 | 0.03435 |
| 6648 | 0.03440 |
| 6248 | 0.03466 |
| phosphorodiamidate | Compound\_1 | 2648 | 0.03467 |
| 4248 | 0.03469 |
| 5648 | 0.03474 |
| 5248 | 0.03489 |
| 6648 | 0.03494 |
| 6248 | 0.03510 |
| Compound\_2 | 4248 | 0.03902 |
| 2248 | 0.03908 |
| 2648 | 0.03913 |
| 5248 | 0.03920 |
| 6648 | 0.03921 |
| 6248 | 0.03941 |
| Compound\_3 | 3648 | 0.03965 |
| 5648 | 0.03972 |
| 2648 | 0.03977 |
| 5248 | 0.03977 |
| 6648 | 0.03988 |
| 6248 | 0.03993 |
| phosphorodiamidite | Compound\_1 | 6448 | 0.04746 |
| 5648 | 0.04747 |
| 6647 | 0.04749 |
| 6248 | 0.04752 |
| 6548 | 0.04757 |
| 6648 | 0.04773 |
| Compound\_2 | 5648 | 0.03749 |
| 6548 | 0.03756 |
| 6647 | 0.03756 |
| 5248 | 0.03758 |
| 6248 | 0.03774 |
| 6648 | 0.03782 |
| Compound\_3 | 6647 | 0.04280 |
| 6448 | 0.04282 |
| 6348 | 0.04285 |
| 6548 | 0.04292 |
| 6248 | 0.04298 |
| 6648 | 0.04308 |
| phosphorotriamidate | Compound\_1 | 4648 | 0.04610 |
| 3648 | 0.04611 |
| 5648 | 0.04617 |
| 6248 | 0.04617 |
| 2648 | 0.04618 |
| 6648 | 0.04629 |
| Compound\_2 | 4648 | 0.04431 |
| 3648 | 0.04434 |
| 5648 | 0.04439 |
| 6248 | 0.04441 |
| 2648 | 0.04445 |
| 6648 | 0.04457 |
| Compound\_3 | 5248 | 0.04146 |
| 3648 | 0.04147 |
| 5648 | 0.04149 |
| 2648 | 0.04161 |
| 6248 | 0.04161 |
| 6648 | 0.04165 |
| phosphorotriamidite | Compound\_1 | 6348 | 0.04041 |
| 6248 | 0.04042 |
| 6448 | 0.04050 |
| 6647 | 0.04053 |
| 6548 | 0.04065 |
| 6648 | 0.04081 |
| Compound\_2 | 5648 | 0.04795 |
| 6348 | 0.04795 |
| 6248 | 0.04796 |
| 6448 | 0.04800 |
| 6548 | 0.04807 |
| 6648 | 0.04814 |
| Compound\_3 | 5648 | 0.04433 |
| 6248 | 0.04441 |
| 6348 | 0.04441 |
| 6448 | 0.04445 |
| 6548 | 0.04451 |
| 6648 | 0.04457 |