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

| **drug** | **compound** | **alphavalue** | **nl** | **RMSD\_MAP** |
| --- | --- | --- | --- | --- |
| Phosphate | Compound\_1 | 3.459 | 4555 | 0.02795 |
| 5555 | 0.02795 |
| 5666 | 0.02801 |
| 6666 | 0.02802 |
| 4455 | 0.02807 |
| 3.600 | 4555 | 0.02795 |
| 5555 | 0.02795 |
| 5666 | 0.02801 |
| 6666 | 0.02802 |
| 4455 | 0.02807 |
| 3.800 | 4555 | 0.02795 |
| 5555 | 0.02795 |
| 5666 | 0.02801 |
| 6666 | 0.02802 |
| 4455 | 0.02807 |
| Compound\_2 | 3.459 | 5566 | 0.03807 |
| 6566 | 0.03809 |
| 4566 | 0.03811 |
| 4455 | 0.03812 |
| 5455 | 0.03814 |
| 3.600 | 5566 | 0.03807 |
| 6566 | 0.03809 |
| 4566 | 0.03811 |
| 4455 | 0.03812 |
| 5455 | 0.03814 |
| 3.800 | 5566 | 0.03807 |
| 6566 | 0.03809 |
| 4566 | 0.03811 |
| 4455 | 0.03812 |
| 5455 | 0.03814 |
| Compound\_3 | 3.459 | 5566 | 0.03388 |
| 4455 | 0.03390 |
| 5567 | 0.03392 |
| 4555 | 0.03393 |
| 4566 | 0.03393 |
| 3.800 | 5566 | 0.03388 |
| 4455 | 0.03390 |
| 5567 | 0.03392 |
| 4555 | 0.03393 |
| 4566 | 0.03393 |
| Phosphinamidate | Compound\_1 | 3.459 | 5556 | 0.03550 |
| 4456 | 0.03552 |
| 4556 | 0.03552 |
| 4445 | 0.03554 |
| 5456 | 0.03554 |
| 3.600 | 5556 | 0.03550 |
| 4456 | 0.03552 |
| 4556 | 0.03552 |
| 4445 | 0.03554 |
| 5456 | 0.03554 |
| 3.800 | 5556 | 0.03550 |
| 4456 | 0.03552 |
| 4556 | 0.03552 |
| 4445 | 0.03554 |
| 5456 | 0.03554 |
| Compound\_2 | 3.459 | 4556 | 0.04467 |
| 3445 | 0.04470 |
| 3556 | 0.04472 |
| 4555 | 0.04472 |
| 5667 | 0.04474 |
| 3.600 | 4556 | 0.04467 |
| 3445 | 0.04470 |
| 3556 | 0.04472 |
| 4555 | 0.04472 |
| 5667 | 0.04474 |
| 3.800 | 4556 | 0.04467 |
| 3445 | 0.04470 |
| 3556 | 0.04472 |
| 4555 | 0.04472 |
| 5667 | 0.04474 |
| Compound\_3 | 3.459 | 4556 | 0.03502 |
| 5556 | 0.03503 |
| 4456 | 0.03506 |
| 3445 | 0.03507 |
| 4445 | 0.03507 |
| 3.600 | 4556 | 0.03502 |
| 5556 | 0.03503 |
| 4456 | 0.03506 |
| 3445 | 0.03507 |
| 4445 | 0.03507 |
| 3.800 | 4556 | 0.03502 |
| 5556 | 0.03503 |
| 4456 | 0.03506 |
| 3445 | 0.03507 |
| 4445 | 0.03507 |
| Phosphinate | Compound\_1 | 3.459 | 5555 | 0.03564 |
| 5556 | 0.03564 |
| 4556 | 0.03565 |
| 4555 | 0.03566 |
| 6666 | 0.03569 |
| 3.600 | 5555 | 0.03564 |
| 5556 | 0.03564 |
| 4556 | 0.03565 |
| 4555 | 0.03566 |
| 6666 | 0.03569 |
| 3.800 | 5555 | 0.03564 |
| 5556 | 0.03564 |
| 4556 | 0.03565 |
| 4555 | 0.03566 |
| 6666 | 0.03569 |
| Compound\_2 | 3.459 | 4556 | 0.03271 |
| 3556 | 0.03277 |
| 4456 | 0.03277 |
| 3445 | 0.03278 |
| 5556 | 0.03278 |
| 3.600 | 4556 | 0.03271 |
| 3556 | 0.03277 |
| 4456 | 0.03277 |
| 3445 | 0.03278 |
| 5556 | 0.03278 |
| 3.800 | 4556 | 0.03271 |
| 3556 | 0.03277 |
| 4456 | 0.03277 |
| 3445 | 0.03278 |
| 5556 | 0.03278 |
| Compound\_3 | 3.459 | 4556 | 0.04244 |
| 4455 | 0.04245 |
| 4456 | 0.04245 |
| 4555 | 0.04245 |
| 5556 | 0.04247 |
| 3.600 | 4556 | 0.04244 |
| 4455 | 0.04245 |
| 4456 | 0.04245 |
| 4555 | 0.04245 |
| 5556 | 0.04247 |
| 3.800 | 4556 | 0.04244 |
| 4455 | 0.04245 |
| 4456 | 0.04245 |
| 4555 | 0.04245 |
| 5556 | 0.04247 |
| Phosphine | Compound\_1 | 3.459 | 2356 | 0.03476 |
| 2467 | 0.03476 |
| 2367 | 0.03477 |
| 2256 | 0.03478 |
| 2357 | 0.03479 |
| 3.600 | 2356 | 0.03476 |
| 2467 | 0.03476 |
| 2367 | 0.03477 |
| 2256 | 0.03478 |
| 2357 | 0.03479 |
| 3.800 | 2356 | 0.03476 |
| 2467 | 0.03476 |
| 2367 | 0.03477 |
| 2256 | 0.03478 |
| 2357 | 0.03479 |
| Compound\_2 | 3.459 | 2356 | 0.03402 |
| 2367 | 0.03402 |
| 2467 | 0.03402 |
| 2256 | 0.03403 |
| 2267 | 0.03406 |
| 3.600 | 2356 | 0.03402 |
| 2367 | 0.03402 |
| 2467 | 0.03402 |
| 2256 | 0.03403 |
| 2267 | 0.03406 |
| 3.800 | 2356 | 0.03402 |
| 2367 | 0.03402 |
| 2467 | 0.03402 |
| 2256 | 0.03403 |
| 2267 | 0.03406 |
| Compound\_3 | 3.459 | 2367 | 0.03892 |
| 2467 | 0.03892 |
| 2468 | 0.03895 |
| 2368 | 0.03897 |
| 2267 | 0.03900 |
| 3.600 | 2367 | 0.03892 |
| 2467 | 0.03892 |
| 2468 | 0.03895 |
| 2368 | 0.03897 |
| 2267 | 0.03900 |
| 3.800 | 2367 | 0.03892 |
| 2467 | 0.03892 |
| 2468 | 0.03895 |
| 2368 | 0.03897 |
| 2267 | 0.03900 |
| PhosphineOxide | Compound\_1 | 3.459 | 4456 | 0.03615 |
| 4556 | 0.03617 |
| 3345 | 0.03618 |
| 3445 | 0.03619 |
| 3456 | 0.03619 |
| 3.600 | 4456 | 0.03615 |
| 4556 | 0.03617 |
| 3345 | 0.03618 |
| 3445 | 0.03619 |
| 3456 | 0.03619 |
| 3.800 | 4456 | 0.03615 |
| 4556 | 0.03617 |
| 3345 | 0.03618 |
| 3445 | 0.03619 |
| 3456 | 0.03619 |
| Compound\_2 | 3.459 | 4445 | 0.04270 |
| 3445 | 0.04272 |
| 4345 | 0.04272 |
| 4456 | 0.04272 |
| 3345 | 0.04273 |
| 3.600 | 4445 | 0.04270 |
| 3445 | 0.04272 |
| 4345 | 0.04272 |
| 4456 | 0.04272 |
| 3345 | 0.04273 |
| 3.800 | 4445 | 0.04270 |
| 3445 | 0.04272 |
| 4345 | 0.04272 |
| 4456 | 0.04272 |
| 3345 | 0.04273 |
| Compound\_3 | 3.459 | 4445 | 0.03665 |
| 5556 | 0.03666 |
| 4556 | 0.03668 |
| 3445 | 0.03669 |
| 5445 | 0.03671 |
| 3.600 | 4445 | 0.03665 |
| 5556 | 0.03666 |
| 4556 | 0.03668 |
| 3445 | 0.03669 |
| 5445 | 0.03671 |
| 3.800 | 4445 | 0.03665 |
| 5556 | 0.03666 |
| 4556 | 0.03668 |
| 3445 | 0.03669 |
| 5445 | 0.03671 |
| Phosphinite | Compound\_1 | 3.459 | 2356 | 0.03220 |
| 2467 | 0.03221 |
| 2456 | 0.03223 |
| 2367 | 0.03227 |
| 2567 | 0.03227 |
| 3.600 | 2356 | 0.03220 |
| 2467 | 0.03221 |
| 2456 | 0.03223 |
| 2367 | 0.03227 |
| 2567 | 0.03227 |
| 3.800 | 2356 | 0.03220 |
| 2467 | 0.03221 |
| 2456 | 0.03223 |
| 2367 | 0.03227 |
| 2567 | 0.03227 |
| Compound\_2 | 3.459 | 2467 | 0.03324 |
| 2367 | 0.03326 |
| 2567 | 0.03328 |
| 2356 | 0.03329 |
| 2267 | 0.03332 |
| 3.600 | 2467 | 0.03324 |
| 2367 | 0.03326 |
| 2567 | 0.03328 |
| 2356 | 0.03329 |
| 2267 | 0.03332 |
| 3.800 | 2467 | 0.03324 |
| 2367 | 0.03326 |
| 2567 | 0.03328 |
| 2356 | 0.03329 |
| 2267 | 0.03332 |
| Compound\_3 | 3.459 | 2356 | 0.03919 |
| 2467 | 0.03922 |
| 2456 | 0.03923 |
| 2367 | 0.03926 |
| 2256 | 0.03927 |
| 3.600 | 2356 | 0.03919 |
| 2467 | 0.03922 |
| 2456 | 0.03923 |
| 2367 | 0.03926 |
| 2256 | 0.03927 |
| 3.800 | 2356 | 0.03919 |
| 2467 | 0.03922 |
| 2456 | 0.03923 |
| 2367 | 0.03926 |
| 2256 | 0.03927 |
| Phosphite | Compound\_1 | 3.459 | 2466 | 0.03736 |
| 2467 | 0.03740 |
| 2366 | 0.03743 |
| 2566 | 0.03745 |
| 2567 | 0.03746 |
| 3.600 | 2466 | 0.03736 |
| 2467 | 0.03740 |
| 2366 | 0.03743 |
| 2566 | 0.03745 |
| 2567 | 0.03746 |
| 3.800 | 2466 | 0.03736 |
| 2467 | 0.03740 |
| 2366 | 0.03743 |
| 2566 | 0.03745 |
| 2567 | 0.03746 |
| Compound\_2 | 3.459 | 2466 | 0.03824 |
| 2467 | 0.03827 |
| 2566 | 0.03828 |
| 2567 | 0.03829 |
| 2366 | 0.03834 |
| 3.600 | 2466 | 0.03824 |
| 2467 | 0.03827 |
| 2566 | 0.03828 |
| 2567 | 0.03829 |
| 2366 | 0.03834 |
| 3.800 | 2466 | 0.03824 |
| 2467 | 0.03827 |
| 2566 | 0.03828 |
| 2567 | 0.03829 |
| 2366 | 0.03834 |
| Compound\_3 | 3.459 | 2456 | 0.03461 |
| 3567 | 0.03462 |
| 2567 | 0.03465 |
| 2556 | 0.03467 |
| 2356 | 0.03468 |
| 3.600 | 2456 | 0.03461 |
| 3567 | 0.03462 |
| 2567 | 0.03465 |
| 2556 | 0.03467 |
| 2356 | 0.03468 |
| 3.800 | 2456 | 0.03461 |
| 3567 | 0.03462 |
| 2567 | 0.03465 |
| 2556 | 0.03467 |
| 2356 | 0.03468 |
| Phosphoamidite | Compound\_1 | 3.459 | 2466 | 0.03932 |
| 2467 | 0.03932 |
| 2567 | 0.03937 |
| 2356 | 0.03940 |
| 2366 | 0.03940 |
| 3.600 | 2466 | 0.03932 |
| 2467 | 0.03932 |
| 2567 | 0.03937 |
| 2356 | 0.03940 |
| 2366 | 0.03940 |
| 3.800 | 2466 | 0.03932 |
| 2467 | 0.03932 |
| 2567 | 0.03937 |
| 2356 | 0.03940 |
| 2366 | 0.03940 |
| Compound\_2 | 3.459 | 2356 | 0.03855 |
| 2456 | 0.03855 |
| 2355 | 0.03856 |
| 2466 | 0.03857 |
| 2455 | 0.03858 |
| 3.600 | 2356 | 0.03855 |
| 2456 | 0.03855 |
| 2355 | 0.03856 |
| 2466 | 0.03857 |
| 2455 | 0.03858 |
| 3.800 | 2356 | 0.03855 |
| 2456 | 0.03855 |
| 2355 | 0.03856 |
| 2466 | 0.03857 |
| 2455 | 0.03858 |
| Compound\_3 | 3.459 | 2466 | 0.03717 |
| 2467 | 0.03720 |
| 2355 | 0.03725 |
| 2566 | 0.03725 |
| 2567 | 0.03725 |
| 3.600 | 2466 | 0.03717 |
| 2467 | 0.03720 |
| 2355 | 0.03725 |
| 2566 | 0.03725 |
| 2567 | 0.03725 |
| 3.800 | 2466 | 0.03717 |
| 2467 | 0.03720 |
| 2355 | 0.03725 |
| 2566 | 0.03725 |
| 2567 | 0.03725 |
| Phosphonamidite | Compound\_1 | 3.459 | 2467 | 0.03685 |
| 2466 | 0.03688 |
| 2567 | 0.03690 |
| 2356 | 0.03693 |
| 2367 | 0.03694 |
| 3.600 | 2467 | 0.03685 |
| 2466 | 0.03688 |
| 2567 | 0.03690 |
| 2356 | 0.03693 |
| 2367 | 0.03694 |
| 3.800 | 2467 | 0.03685 |
| 2466 | 0.03688 |
| 2567 | 0.03690 |
| 2356 | 0.03693 |
| 2367 | 0.03694 |
| Compound\_2 | 3.459 | 2467 | 0.03947 |
| 2356 | 0.03948 |
| 2367 | 0.03949 |
| 2466 | 0.03950 |
| 2366 | 0.03951 |
| 3.600 | 2467 | 0.03947 |
| 2356 | 0.03948 |
| 2367 | 0.03949 |
| 2466 | 0.03950 |
| 2366 | 0.03951 |
| 3.800 | 2467 | 0.03947 |
| 2356 | 0.03948 |
| 2367 | 0.03949 |
| 2466 | 0.03950 |
| 2366 | 0.03951 |
| Compound\_3 | 3.459 | 2467 | 0.03262 |
| 2466 | 0.03263 |
| 2567 | 0.03267 |
| 2366 | 0.03269 |
| 2356 | 0.03270 |
| 3.600 | 2467 | 0.03262 |
| 2466 | 0.03263 |
| 2567 | 0.03267 |
| 2366 | 0.03269 |
| 2356 | 0.03270 |
| 3.800 | 2467 | 0.03262 |
| 2466 | 0.03263 |
| 2567 | 0.03267 |
| 2366 | 0.03269 |
| 2356 | 0.03270 |
| Phosphonate | Compound\_1 | 3.459 | 5555 | 0.02976 |
| 5556 | 0.02978 |
| 4555 | 0.02979 |
| 6666 | 0.02979 |
| 6667 | 0.02980 |
| 3.600 | 5555 | 0.02976 |
| 5556 | 0.02978 |
| 4555 | 0.02979 |
| 6666 | 0.02979 |
| 6667 | 0.02980 |
| 3.800 | 5555 | 0.02976 |
| 5556 | 0.02978 |
| 4555 | 0.02979 |
| 6666 | 0.02979 |
| 6667 | 0.02980 |
| Compound\_2 | 3.459 | 5555 | 0.03060 |
| 4555 | 0.03063 |
| 5556 | 0.03065 |
| 4556 | 0.03067 |
| 5666 | 0.03067 |
| 3.600 | 5555 | 0.03060 |
| 4555 | 0.03063 |
| 5556 | 0.03065 |
| 4556 | 0.03067 |
| 5666 | 0.03067 |
| 3.800 | 5555 | 0.03060 |
| 4555 | 0.03063 |
| 5556 | 0.03065 |
| 4556 | 0.03067 |
| 5666 | 0.03067 |
| Compound\_3 | 3.459 | 4556 | 0.03271 |
| 4456 | 0.03274 |
| 3445 | 0.03276 |
| 3456 | 0.03276 |
| 3556 | 0.03276 |
| 3.600 | 4556 | 0.03271 |
| 4456 | 0.03274 |
| 3445 | 0.03276 |
| 3456 | 0.03276 |
| 3556 | 0.03276 |
| 3.800 | 4556 | 0.03271 |
| 4456 | 0.03274 |
| 3445 | 0.03276 |
| 3456 | 0.03276 |
| 3556 | 0.03276 |
| Phosphondiamidate | Compound\_1 | 3.459 | 4556 | 0.03641 |
| 4456 | 0.03643 |
| 3456 | 0.03645 |
| 3556 | 0.03646 |
| 5556 | 0.03647 |
| 3.600 | 4556 | 0.03641 |
| 4456 | 0.03643 |
| 3456 | 0.03645 |
| 3556 | 0.03646 |
| 5556 | 0.03647 |
| 3.800 | 4556 | 0.03641 |
| 4456 | 0.03643 |
| 3456 | 0.03645 |
| 3556 | 0.03646 |
| 5556 | 0.03647 |
| Compound\_2 | 3.459 | 4556 | 0.03715 |
| 5556 | 0.03715 |
| 4456 | 0.03716 |
| 5567 | 0.03718 |
| 5456 | 0.03719 |
| 3.600 | 4556 | 0.03715 |
| 5556 | 0.03715 |
| 4456 | 0.03716 |
| 5567 | 0.03718 |
| 5456 | 0.03719 |
| 3.800 | 4556 | 0.03715 |
| 5556 | 0.03715 |
| 4456 | 0.03716 |
| 5567 | 0.03718 |
| 5456 | 0.03719 |
| Compound\_3 | 3.459 | 4456 | 0.04306 |
| 5556 | 0.04308 |
| 4556 | 0.04309 |
| 5456 | 0.04309 |
| 5567 | 0.04310 |
| 3.600 | 4456 | 0.04306 |
| 5556 | 0.04308 |
| 4556 | 0.04309 |
| 5456 | 0.04309 |
| 5567 | 0.04310 |
| 3.800 | 4456 | 0.04306 |
| 5556 | 0.04308 |
| 4556 | 0.04309 |
| 5456 | 0.04309 |
| 5567 | 0.04310 |
| Phosphonite | Compound\_1 | 3.459 | 2467 | 0.03928 |
| 2466 | 0.03929 |
| 2567 | 0.03930 |
| 2566 | 0.03933 |
| 2456 | 0.03934 |
| 3.600 | 2467 | 0.03928 |
| 2466 | 0.03929 |
| 2567 | 0.03930 |
| 2566 | 0.03933 |
| 2456 | 0.03934 |
| 3.800 | 2467 | 0.03928 |
| 2466 | 0.03929 |
| 2567 | 0.03930 |
| 2566 | 0.03933 |
| 2456 | 0.03934 |
| Compound\_2 | 3.459 | 2456 | 0.03379 |
| 2467 | 0.03381 |
| 2567 | 0.03381 |
| 2356 | 0.03387 |
| 2466 | 0.03388 |
| 3.600 | 2456 | 0.03379 |
| 2467 | 0.03381 |
| 2567 | 0.03381 |
| 2356 | 0.03387 |
| 2466 | 0.03388 |
| 3.800 | 2456 | 0.03379 |
| 2467 | 0.03381 |
| 2567 | 0.03381 |
| 2356 | 0.03387 |
| 2466 | 0.03388 |
| Compound\_3 | 3.459 | 2466 | 0.03229 |
| 2566 | 0.03229 |
| 2567 | 0.03230 |
| 2455 | 0.03231 |
| 2456 | 0.03231 |
| 3.600 | 2466 | 0.03229 |
| 2566 | 0.03229 |
| 2567 | 0.03230 |
| 2455 | 0.03231 |
| 2456 | 0.03231 |
| 3.800 | 2466 | 0.03229 |
| 2566 | 0.03229 |
| 2567 | 0.03230 |
| 2455 | 0.03231 |
| 2456 | 0.03231 |
| Phosphonodiamidite | Compound\_1 | 3.459 | 2356 | 0.04686 |
| 2367 | 0.04686 |
| 2467 | 0.04686 |
| 2256 | 0.04687 |
| 2267 | 0.04690 |
| 3.600 | 2356 | 0.04686 |
| 2367 | 0.04686 |
| 2467 | 0.04686 |
| 2256 | 0.04687 |
| 2267 | 0.04690 |
| 3.800 | 2356 | 0.04686 |
| 2367 | 0.04686 |
| 2467 | 0.04686 |
| 2256 | 0.04687 |
| 2267 | 0.04690 |
| Compound\_2 | 3.459 | 2367 | 0.04129 |
| 2467 | 0.04129 |
| 2366 | 0.04131 |
| 2356 | 0.04132 |
| 2466 | 0.04132 |
| 3.600 | 2367 | 0.04129 |
| 2467 | 0.04129 |
| 2366 | 0.04131 |
| 2356 | 0.04132 |
| 2466 | 0.04132 |
| 3.800 | 2367 | 0.04129 |
| 2467 | 0.04129 |
| 2366 | 0.04131 |
| 2356 | 0.04132 |
| 2466 | 0.04132 |
| Compound\_3 | 3.459 | 2467 | 0.03749 |
| 2567 | 0.03752 |
| 2356 | 0.03754 |
| 2456 | 0.03754 |
| 2466 | 0.03754 |
| 3.600 | 2467 | 0.03749 |
| 2567 | 0.03752 |
| 2356 | 0.03754 |
| 2456 | 0.03754 |
| 2466 | 0.03754 |
| 3.800 | 2467 | 0.03749 |
| 2567 | 0.03752 |
| 2356 | 0.03754 |
| 2456 | 0.03754 |
| 2466 | 0.03754 |
| Phosphoroamidate | Compound\_1 | 3.459 | 4556 | 0.03643 |
| 4555 | 0.03645 |
| 5667 | 0.03645 |
| 4456 | 0.03646 |
| 5567 | 0.03646 |
| 3.600 | 4556 | 0.03643 |
| 4555 | 0.03645 |
| 5667 | 0.03645 |
| 4456 | 0.03646 |
| 5567 | 0.03646 |
| 3.800 | 4556 | 0.03643 |
| 4555 | 0.03645 |
| 5667 | 0.03645 |
| 4456 | 0.03646 |
| 5567 | 0.03646 |
| Compound\_2 | 3.459 | 5667 | 0.04096 |
| 5567 | 0.04097 |
| 5566 | 0.04099 |
| 5666 | 0.04099 |
| 4556 | 0.04100 |
| 3.600 | 5667 | 0.04096 |
| 5567 | 0.04097 |
| 5566 | 0.04099 |
| 5666 | 0.04099 |
| 4556 | 0.04100 |
| Compound\_3 | 3.459 | 5667 | 0.03130 |
| 4556 | 0.03132 |
| 5666 | 0.03132 |
| 4555 | 0.03133 |
| 5567 | 0.03134 |
| 3.600 | 5667 | 0.03130 |
| 4556 | 0.03132 |
| 5666 | 0.03132 |
| 4555 | 0.03133 |
| 5567 | 0.03134 |
| 3.800 | 5667 | 0.03130 |
| 4556 | 0.03132 |
| 5666 | 0.03132 |
| 4555 | 0.03133 |
| 5567 | 0.03134 |
| Phosphorodiamidate | Compound\_1 | 3.459 | 4456 | 0.03214 |
| 4556 | 0.03215 |
| 4567 | 0.03215 |
| 3456 | 0.03216 |
| 5567 | 0.03216 |
| 3.600 | 4456 | 0.03214 |
| 4556 | 0.03215 |
| 4567 | 0.03215 |
| 3456 | 0.03216 |
| 5567 | 0.03216 |
| 3.800 | 4456 | 0.03214 |
| 4556 | 0.03215 |
| 4567 | 0.03215 |
| 3456 | 0.03216 |
| 5567 | 0.03216 |
| Compound\_2 | 3.459 | 4456 | 0.03658 |
| 5567 | 0.03658 |
| 4556 | 0.03659 |
| 4567 | 0.03662 |
| 5667 | 0.03662 |
| 3.600 | 4456 | 0.03658 |
| 5567 | 0.03658 |
| 4556 | 0.03659 |
| 4567 | 0.03662 |
| 5667 | 0.03662 |
| 3.800 | 4456 | 0.03658 |
| 5567 | 0.03658 |
| 4556 | 0.03659 |
| 4567 | 0.03662 |
| 5667 | 0.03662 |
| Compound\_3 | 3.459 | 4456 | 0.03718 |
| 5567 | 0.03721 |
| 3456 | 0.03723 |
| 4556 | 0.03723 |
| 4567 | 0.03723 |
| 3.600 | 4456 | 0.03718 |
| 5567 | 0.03721 |
| 3456 | 0.03723 |
| 4556 | 0.03723 |
| 4567 | 0.03723 |
| 3.800 | 4456 | 0.03718 |
| 5567 | 0.03721 |
| 3456 | 0.03723 |
| 4556 | 0.03723 |
| 4567 | 0.03723 |
| Phosphorodiamidtite | Compound\_1 | 3.459 | 2467 | 0.04538 |
| 2466 | 0.04540 |
| 2567 | 0.04542 |
| 2356 | 0.04545 |
| 2366 | 0.04545 |
| 3.600 | 2467 | 0.04538 |
| 2466 | 0.04540 |
| 2567 | 0.04542 |
| 2356 | 0.04545 |
| 2366 | 0.04545 |
| 3.800 | 2467 | 0.04538 |
| 2466 | 0.04540 |
| 2567 | 0.04542 |
| 2356 | 0.04545 |
| 2366 | 0.04545 |
| Compound\_2 | 3.459 | 2466 | 0.03501 |
| 2467 | 0.03503 |
| 2567 | 0.03504 |
| 2566 | 0.03507 |
| 2456 | 0.03508 |
| 3.600 | 2466 | 0.03501 |
| 2467 | 0.03503 |
| 2567 | 0.03504 |
| 2566 | 0.03507 |
| 2456 | 0.03508 |
| 3.800 | 2466 | 0.03501 |
| 2467 | 0.03503 |
| 2567 | 0.03504 |
| 2566 | 0.03507 |
| 2456 | 0.03508 |
| Compound\_3 | 3.459 | 2467 | 0.04049 |
| 2567 | 0.04049 |
| 2456 | 0.04051 |
| 2466 | 0.04052 |
| 2356 | 0.04054 |
| 3.600 | 2467 | 0.04049 |
| 2567 | 0.04049 |
| 2456 | 0.04051 |
| 2466 | 0.04052 |
| 2356 | 0.04054 |
| 3.800 | 2467 | 0.04049 |
| 2567 | 0.04049 |
| 2456 | 0.04051 |
| 2466 | 0.04052 |
| 2356 | 0.04054 |
| Phosphorotriamidate | Compound\_1 | 3.459 | 4456 | 0.04457 |
| 4556 | 0.04457 |
| 5456 | 0.04460 |
| 4445 | 0.04461 |
| 3445 | 0.04462 |
| 3.600 | 4456 | 0.04450 |
| 4556 | 0.04450 |
| 4445 | 0.04453 |
| 5456 | 0.04453 |
| 3445 | 0.04454 |
| 3.800 | 4456 | 0.04457 |
| 4556 | 0.04457 |
| 5456 | 0.04460 |
| 3445 | 0.04461 |
| 4445 | 0.04461 |
| Compound\_2 | 3.459 | 4456 | 0.04254 |
| 5456 | 0.04256 |
| 5567 | 0.04256 |
| 6567 | 0.04258 |
| 3456 | 0.04260 |
| 3.600 | 4456 | 0.04254 |
| 5456 | 0.04256 |
| 5567 | 0.04256 |
| 6567 | 0.04258 |
| 3456 | 0.04260 |
| 3.800 | 4456 | 0.04254 |
| 5456 | 0.04256 |
| 5567 | 0.04256 |
| 6567 | 0.04258 |
| 3456 | 0.04260 |
| Compound\_3 | 3.459 | 4456 | 0.03951 |
| 5567 | 0.03954 |
| 3456 | 0.03955 |
| 4556 | 0.03956 |
| 4567 | 0.03956 |
| 3.800 | 4456 | 0.03951 |
| 5567 | 0.03954 |
| 3456 | 0.03955 |
| 4556 | 0.03956 |
| 4567 | 0.03956 |
| Phosphorotriamidite | Compound\_1 | 3.459 | 2367 | 0.03765 |
| 2356 | 0.03767 |
| 2467 | 0.03767 |
| 2256 | 0.03768 |
| 2366 | 0.03768 |
| 3.600 | 2367 | 0.03765 |
| 2356 | 0.03767 |
| 2467 | 0.03767 |
| 2256 | 0.03768 |
| 2366 | 0.03768 |
| 3.800 | 2367 | 0.03765 |
| 2356 | 0.03767 |
| 2467 | 0.03767 |
| 2256 | 0.03768 |
| 2366 | 0.03768 |
| Compound\_2 | 3.459 | 2367 | 0.04619 |
| 2256 | 0.04620 |
| 2356 | 0.04620 |
| 2467 | 0.04621 |
| 2267 | 0.04622 |
| 3.600 | 2367 | 0.04619 |
| 2256 | 0.04620 |
| 2356 | 0.04620 |
| 2467 | 0.04621 |
| 2267 | 0.04622 |
| 3.800 | 2367 | 0.04619 |
| 2256 | 0.04620 |
| 2356 | 0.04620 |
| 2467 | 0.04621 |
| 2267 | 0.04622 |
| Compound\_3 | 3.459 | 2256 | 0.04260 |
| 2356 | 0.04260 |
| 2367 | 0.04262 |
| 2467 | 0.04264 |
| 2267 | 0.04265 |
| 3.600 | 2256 | 0.04260 |
| 2356 | 0.04260 |
| 2367 | 0.04262 |
| 2467 | 0.04264 |
| 2267 | 0.04265 |
| 3.800 | 2256 | 0.04260 |
| 2356 | 0.04260 |
| 2367 | 0.04262 |
| 2467 | 0.04264 |
| 2267 | 0.04265 |

## 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 |
| 3.600 | 2248 | 0.03120 |
| 4248 | 0.03133 |
| 6247 | 0.03134 |
| 6258 | 0.03137 |
| 5248 | 0.03164 |
| 6248 | 0.03198 |
| 3.800 | 2248 | 0.03120 |
| 4248 | 0.03133 |
| 6247 | 0.03134 |
| 6258 | 0.03137 |
| 5248 | 0.03164 |
| 6248 | 0.03198 |
| Compound\_2 | 3.459 | 3648 | 0.04079 |
| 5648 | 0.04079 |
| 5248 | 0.04088 |
| 2648 | 0.04093 |
| 6648 | 0.04093 |
| 6248 | 0.04103 |
| 3.600 | 3648 | 0.04079 |
| 5648 | 0.04079 |
| 5248 | 0.04088 |
| 2648 | 0.04093 |
| 6648 | 0.04093 |
| 6248 | 0.04103 |
| 3.800 | 3648 | 0.04079 |
| 5648 | 0.04079 |
| 5248 | 0.04088 |
| 2648 | 0.04093 |
| 6648 | 0.04093 |
| 6248 | 0.04103 |
| Compound\_3 | 3.459 | 2248 | 0.03663 |
| 5648 | 0.03663 |
| 5248 | 0.03685 |
| 2648 | 0.03686 |
| 6648 | 0.03689 |
| 6248 | 0.03715 |
| 3.800 | 2248 | 0.03663 |
| 5648 | 0.03663 |
| 5248 | 0.03685 |
| 2648 | 0.03686 |
| 6648 | 0.03689 |
| 6248 | 0.03715 |
| Phosphinamidate | Compound\_1 | 3.459 | 5248 | 0.03714 |
| 6548 | 0.03715 |
| 5648 | 0.03719 |
| 2648 | 0.03722 |
| 6248 | 0.03724 |
| 6648 | 0.03738 |
| 3.600 | 5248 | 0.03714 |
| 6548 | 0.03715 |
| 5648 | 0.03719 |
| 2648 | 0.03722 |
| 6248 | 0.03724 |
| 6648 | 0.03738 |
| 3.800 | 5248 | 0.03714 |
| 6548 | 0.03715 |
| 5648 | 0.03719 |
| 2648 | 0.03722 |
| 6248 | 0.03724 |
| 6648 | 0.03738 |
| Compound\_2 | 3.459 | 5265 | 0.04644 |
| 4248 | 0.04650 |
| 6265 | 0.04653 |
| 5248 | 0.04663 |
| 6648 | 0.04663 |
| 6248 | 0.04671 |
| 3.600 | 5265 | 0.04644 |
| 4248 | 0.04650 |
| 6265 | 0.04653 |
| 5248 | 0.04663 |
| 6648 | 0.04663 |
| 6248 | 0.04671 |
| 3.800 | 5265 | 0.04644 |
| 4248 | 0.04650 |
| 6265 | 0.04653 |
| 5248 | 0.04663 |
| 6648 | 0.04663 |
| 6248 | 0.04671 |
| Compound\_3 | 3.459 | 6548 | 0.03671 |
| 2648 | 0.03676 |
| 5648 | 0.03676 |
| 5248 | 0.03680 |
| 6248 | 0.03692 |
| 6648 | 0.03699 |
| 3.600 | 6548 | 0.03671 |
| 2648 | 0.03676 |
| 5648 | 0.03676 |
| 5248 | 0.03680 |
| 6248 | 0.03692 |
| 6648 | 0.03699 |
| 3.800 | 6548 | 0.03671 |
| 2648 | 0.03676 |
| 5648 | 0.03676 |
| 5248 | 0.03680 |
| 6248 | 0.03692 |
| 6648 | 0.03699 |
| Phosphinate | Compound\_1 | 3.459 | 4248 | 0.03739 |
| 3248 | 0.03741 |
| 2648 | 0.03747 |
| 5248 | 0.03748 |
| 2248 | 0.03755 |
| 6248 | 0.03765 |
| 3.600 | 4248 | 0.03739 |
| 3248 | 0.03741 |
| 2648 | 0.03747 |
| 5248 | 0.03748 |
| 2248 | 0.03755 |
| 6248 | 0.03765 |
| 3.800 | 4248 | 0.03739 |
| 3248 | 0.03741 |
| 2648 | 0.03747 |
| 5248 | 0.03748 |
| 2248 | 0.03755 |
| 6248 | 0.03765 |
| Compound\_2 | 3.459 | 2265 | 0.03492 |
| 2248 | 0.03493 |
| 4248 | 0.03493 |
| 6648 | 0.03500 |
| 5248 | 0.03509 |
| 6248 | 0.03525 |
| 3.600 | 2265 | 0.03492 |
| 2248 | 0.03493 |
| 4248 | 0.03493 |
| 6648 | 0.03500 |
| 5248 | 0.03509 |
| 6248 | 0.03525 |
| 3.800 | 2265 | 0.03492 |
| 2248 | 0.03493 |
| 4248 | 0.03493 |
| 6648 | 0.03500 |
| 5248 | 0.03509 |
| 6248 | 0.03525 |
| Compound\_3 | 3.459 | 5648 | 0.04413 |
| 2248 | 0.04414 |
| 2648 | 0.04421 |
| 5248 | 0.04425 |
| 6648 | 0.04430 |
| 6248 | 0.04439 |
| 3.600 | 5648 | 0.04413 |
| 2248 | 0.04414 |
| 2648 | 0.04421 |
| 5248 | 0.04425 |
| 6648 | 0.04430 |
| 6248 | 0.04439 |
| 3.800 | 5648 | 0.04413 |
| 2248 | 0.04414 |
| 2648 | 0.04421 |
| 5248 | 0.04425 |
| 6648 | 0.04430 |
| 6248 | 0.04439 |
| Phosphine | Compound\_1 | 3.459 | 5548 | 0.03619 |
| 6448 | 0.03619 |
| 6647 | 0.03620 |
| 5648 | 0.03631 |
| 6548 | 0.03631 |
| 6648 | 0.03642 |
| 3.600 | 5548 | 0.03619 |
| 6448 | 0.03619 |
| 6647 | 0.03620 |
| 5648 | 0.03631 |
| 6548 | 0.03631 |
| 6648 | 0.03642 |
| 3.800 | 5548 | 0.03619 |
| 6448 | 0.03619 |
| 6647 | 0.03620 |
| 5648 | 0.03631 |
| 6548 | 0.03631 |
| 6648 | 0.03642 |
| Compound\_2 | 3.459 | 6448 | 0.03559 |
| 6647 | 0.03560 |
| 5548 | 0.03562 |
| 6548 | 0.03572 |
| 5648 | 0.03574 |
| 6648 | 0.03584 |
| 3.600 | 6448 | 0.03559 |
| 6647 | 0.03560 |
| 5548 | 0.03562 |
| 6548 | 0.03572 |
| 5648 | 0.03574 |
| 6648 | 0.03584 |
| 3.800 | 6448 | 0.03559 |
| 6647 | 0.03560 |
| 5548 | 0.03562 |
| 6548 | 0.03572 |
| 5648 | 0.03574 |
| 6648 | 0.03584 |
| Compound\_3 | 3.459 | 5646 | 0.04078 |
| 5548 | 0.04083 |
| 6548 | 0.04088 |
| 5647 | 0.04093 |
| 5648 | 0.04102 |
| 6648 | 0.04112 |
| 3.600 | 5646 | 0.04078 |
| 5548 | 0.04083 |
| 6548 | 0.04088 |
| 5647 | 0.04093 |
| 5648 | 0.04102 |
| 6648 | 0.04112 |
| 3.800 | 5646 | 0.04078 |
| 5548 | 0.04083 |
| 6548 | 0.04088 |
| 5647 | 0.04093 |
| 5648 | 0.04102 |
| 6648 | 0.04112 |
| PhosphineOxide | Compound\_1 | 3.459 | 2648 | 0.03738 |
| 6548 | 0.03738 |
| 5648 | 0.03743 |
| 6647 | 0.03743 |
| 6248 | 0.03747 |
| 6648 | 0.03767 |
| 3.600 | 2648 | 0.03738 |
| 6548 | 0.03738 |
| 5648 | 0.03743 |
| 6647 | 0.03743 |
| 6248 | 0.03747 |
| 6648 | 0.03767 |
| 3.800 | 2648 | 0.03738 |
| 6548 | 0.03738 |
| 5648 | 0.03743 |
| 6647 | 0.03743 |
| 6248 | 0.03747 |
| 6648 | 0.03767 |
| Compound\_2 | 3.459 | 2248 | 0.04358 |
| 5648 | 0.04358 |
| 6248 | 0.04360 |
| 3648 | 0.04361 |
| 2648 | 0.04369 |
| 6648 | 0.04369 |
| 3.600 | 2248 | 0.04358 |
| 5648 | 0.04358 |
| 6248 | 0.04360 |
| 3648 | 0.04361 |
| 2648 | 0.04369 |
| 6648 | 0.04369 |
| 3.800 | 2248 | 0.04358 |
| 5648 | 0.04358 |
| 6248 | 0.04360 |
| 3648 | 0.04361 |
| 2648 | 0.04369 |
| 6648 | 0.04369 |
| Compound\_3 | 3.459 | 4248 | 0.03797 |
| 2648 | 0.03800 |
| 2248 | 0.03801 |
| 5248 | 0.03803 |
| 6648 | 0.03803 |
| 6248 | 0.03808 |
| 3.600 | 4248 | 0.03797 |
| 2648 | 0.03800 |
| 2248 | 0.03801 |
| 5248 | 0.03803 |
| 6648 | 0.03803 |
| 6248 | 0.03808 |
| 3.800 | 4248 | 0.03797 |
| 2648 | 0.03800 |
| 2248 | 0.03801 |
| 5248 | 0.03803 |
| 6648 | 0.03803 |
| 6248 | 0.03808 |
| Phosphinite | Compound\_1 | 3.459 | 6248 | 0.03423 |
| 6448 | 0.03423 |
| 6647 | 0.03434 |
| 5648 | 0.03437 |
| 6548 | 0.03439 |
| 6648 | 0.03458 |
| 3.600 | 6248 | 0.03423 |
| 6448 | 0.03423 |
| 6647 | 0.03434 |
| 5648 | 0.03437 |
| 6548 | 0.03439 |
| 6648 | 0.03458 |
| 3.800 | 6248 | 0.03423 |
| 6448 | 0.03423 |
| 6647 | 0.03434 |
| 5648 | 0.03437 |
| 6548 | 0.03439 |
| 6648 | 0.03458 |
| Compound\_2 | 3.459 | 5648 | 0.03554 |
| 6348 | 0.03557 |
| 6448 | 0.03559 |
| 6248 | 0.03561 |
| 6548 | 0.03569 |
| 6648 | 0.03582 |
| 3.600 | 5648 | 0.03554 |
| 6348 | 0.03557 |
| 6448 | 0.03559 |
| 6248 | 0.03561 |
| 6548 | 0.03569 |
| 6648 | 0.03582 |
| 3.800 | 5648 | 0.03554 |
| 6348 | 0.03557 |
| 6448 | 0.03559 |
| 6248 | 0.03561 |
| 6548 | 0.03569 |
| 6648 | 0.03582 |
| Compound\_3 | 3.459 | 5647 | 0.04095 |
| 6448 | 0.04097 |
| 6647 | 0.04111 |
| 5648 | 0.04113 |
| 6548 | 0.04114 |
| 6648 | 0.04133 |
| 3.600 | 5647 | 0.04095 |
| 6448 | 0.04097 |
| 6647 | 0.04111 |
| 5648 | 0.04113 |
| 6548 | 0.04114 |
| 6648 | 0.04133 |
| 3.800 | 5647 | 0.04095 |
| 6448 | 0.04097 |
| 6647 | 0.04111 |
| 5648 | 0.04113 |
| 6548 | 0.04114 |
| 6648 | 0.04133 |
| Phosphite | Compound\_1 | 3.459 | 5548 | 0.04045 |
| 6647 | 0.04046 |
| 4648 | 0.04061 |
| 6548 | 0.04066 |
| 5648 | 0.04080 |
| 6648 | 0.04095 |
| 3.600 | 5548 | 0.04045 |
| 6647 | 0.04046 |
| 4648 | 0.04061 |
| 6548 | 0.04066 |
| 5648 | 0.04080 |
| 6648 | 0.04095 |
| 3.800 | 5548 | 0.04045 |
| 6647 | 0.04046 |
| 4648 | 0.04061 |
| 6548 | 0.04066 |
| 5648 | 0.04080 |
| 6648 | 0.04095 |
| Compound\_2 | 3.459 | 6647 | 0.04094 |
| 6448 | 0.04096 |
| 5648 | 0.04106 |
| 6248 | 0.04106 |
| 6548 | 0.04111 |
| 6648 | 0.04133 |
| 3.600 | 6647 | 0.04094 |
| 6448 | 0.04096 |
| 5648 | 0.04106 |
| 6248 | 0.04106 |
| 6548 | 0.04111 |
| 6648 | 0.04133 |
| 3.800 | 6647 | 0.04094 |
| 6448 | 0.04096 |
| 5648 | 0.04106 |
| 6248 | 0.04106 |
| 6548 | 0.04111 |
| 6648 | 0.04133 |
| Compound\_3 | 3.459 | 6247 | 0.03740 |
| 6448 | 0.03752 |
| 6548 | 0.03752 |
| 6648 | 0.03759 |
| 6348 | 0.03762 |
| 6248 | 0.03778 |
| 3.600 | 6247 | 0.03740 |
| 6448 | 0.03752 |
| 6548 | 0.03752 |
| 6648 | 0.03759 |
| 6348 | 0.03762 |
| 6248 | 0.03778 |
| 3.800 | 6247 | 0.03740 |
| 6448 | 0.03752 |
| 6548 | 0.03752 |
| 6648 | 0.03759 |
| 6348 | 0.03762 |
| 6248 | 0.03778 |
| Phosphoamidite | Compound\_1 | 3.459 | 6448 | 0.04170 |
| 6647 | 0.04179 |
| 6248 | 0.04181 |
| 6548 | 0.04188 |
| 5648 | 0.04192 |
| 6648 | 0.04212 |
| 3.600 | 6448 | 0.04170 |
| 6647 | 0.04179 |
| 6248 | 0.04181 |
| 6548 | 0.04188 |
| 5648 | 0.04192 |
| 6648 | 0.04212 |
| 3.800 | 6448 | 0.04170 |
| 6647 | 0.04179 |
| 6248 | 0.04181 |
| 6548 | 0.04188 |
| 5648 | 0.04192 |
| 6648 | 0.04212 |
| Compound\_2 | 3.459 | 6647 | 0.04101 |
| 6348 | 0.04106 |
| 6448 | 0.04107 |
| 6248 | 0.04114 |
| 6548 | 0.04118 |
| 6648 | 0.04134 |
| 3.600 | 6647 | 0.04101 |
| 6348 | 0.04106 |
| 6448 | 0.04107 |
| 6248 | 0.04114 |
| 6548 | 0.04118 |
| 6648 | 0.04134 |
| 3.800 | 6647 | 0.04101 |
| 6348 | 0.04106 |
| 6448 | 0.04107 |
| 6248 | 0.04114 |
| 6548 | 0.04118 |
| 6648 | 0.04134 |
| Compound\_3 | 3.459 | 5548 | 0.03960 |
| 6647 | 0.03963 |
| 6248 | 0.03965 |
| 6548 | 0.03977 |
| 5648 | 0.03983 |
| 6648 | 0.04001 |
| 3.600 | 5548 | 0.03960 |
| 6647 | 0.03963 |
| 6248 | 0.03965 |
| 6548 | 0.03977 |
| 5648 | 0.03983 |
| 6648 | 0.04001 |
| 3.800 | 5548 | 0.03960 |
| 6647 | 0.03963 |
| 6248 | 0.03965 |
| 6548 | 0.03977 |
| 5648 | 0.03983 |
| 6648 | 0.04001 |
| Phosphonamidite | Compound\_1 | 3.459 | 6448 | 0.03916 |
| 6248 | 0.03922 |
| 6647 | 0.03926 |
| 5648 | 0.03932 |
| 6548 | 0.03933 |
| 6648 | 0.03955 |
| 3.600 | 6448 | 0.03916 |
| 6248 | 0.03922 |
| 6647 | 0.03926 |
| 5648 | 0.03932 |
| 6548 | 0.03933 |
| 6648 | 0.03955 |
| 3.800 | 6448 | 0.03916 |
| 6248 | 0.03922 |
| 6647 | 0.03926 |
| 5648 | 0.03932 |
| 6548 | 0.03933 |
| 6648 | 0.03955 |
| Compound\_2 | 3.459 | 5647 | 0.04145 |
| 5548 | 0.04149 |
| 6647 | 0.04153 |
| 6548 | 0.04161 |
| 5648 | 0.04168 |
| 6648 | 0.04181 |
| 3.600 | 5647 | 0.04145 |
| 5548 | 0.04149 |
| 6647 | 0.04153 |
| 6548 | 0.04161 |
| 5648 | 0.04168 |
| 6648 | 0.04181 |
| 3.800 | 5647 | 0.04145 |
| 5548 | 0.04149 |
| 6647 | 0.04153 |
| 6548 | 0.04161 |
| 5648 | 0.04168 |
| 6648 | 0.04181 |
| Compound\_3 | 3.459 | 6248 | 0.03527 |
| 6448 | 0.03528 |
| 6647 | 0.03534 |
| 5648 | 0.03538 |
| 6548 | 0.03545 |
| 6648 | 0.03567 |
| 3.600 | 6248 | 0.03527 |
| 6448 | 0.03528 |
| 6647 | 0.03534 |
| 5648 | 0.03538 |
| 6548 | 0.03545 |
| 6648 | 0.03567 |
| 3.800 | 6248 | 0.03527 |
| 6448 | 0.03528 |
| 6647 | 0.03534 |
| 5648 | 0.03538 |
| 6548 | 0.03545 |
| 6648 | 0.03567 |
| Phosphonate | Compound\_1 | 3.459 | 2648 | 0.03232 |
| 4248 | 0.03245 |
| 3248 | 0.03247 |
| 5248 | 0.03253 |
| 2248 | 0.03256 |
| 6248 | 0.03264 |
| 3.600 | 2648 | 0.03232 |
| 4248 | 0.03245 |
| 3248 | 0.03247 |
| 5248 | 0.03253 |
| 2248 | 0.03257 |
| 6248 | 0.03264 |
| 3.800 | 2648 | 0.03232 |
| 4248 | 0.03245 |
| 3248 | 0.03247 |
| 5248 | 0.03253 |
| 2248 | 0.03256 |
| 6248 | 0.03264 |
| Compound\_2 | 3.459 | 6348 | 0.03295 |
| 2248 | 0.03302 |
| 4248 | 0.03302 |
| 6247 | 0.03304 |
| 5248 | 0.03327 |
| 6248 | 0.03357 |
| 3.600 | 6348 | 0.03295 |
| 2248 | 0.03302 |
| 4248 | 0.03302 |
| 6247 | 0.03304 |
| 5248 | 0.03327 |
| 6248 | 0.03357 |
| 3.800 | 6348 | 0.03295 |
| 2248 | 0.03302 |
| 4248 | 0.03302 |
| 6247 | 0.03304 |
| 5248 | 0.03327 |
| 6248 | 0.03357 |
| Compound\_3 | 3.459 | 5648 | 0.03491 |
| 2648 | 0.03492 |
| 6348 | 0.03493 |
| 5248 | 0.03509 |
| 6648 | 0.03513 |
| 6248 | 0.03527 |
| 3.600 | 5648 | 0.03491 |
| 2648 | 0.03492 |
| 6348 | 0.03493 |
| 5248 | 0.03509 |
| 6648 | 0.03513 |
| 6248 | 0.03527 |
| 3.800 | 5648 | 0.03491 |
| 2648 | 0.03492 |
| 6348 | 0.03493 |
| 5248 | 0.03509 |
| 6648 | 0.03513 |
| 6248 | 0.03527 |
| Phosphondiamidate | Compound\_1 | 3.459 | 5648 | 0.03831 |
| 6548 | 0.03835 |
| 6348 | 0.03837 |
| 5248 | 0.03841 |
| 6648 | 0.03852 |
| 6248 | 0.03858 |
| 3.600 | 5648 | 0.03831 |
| 6548 | 0.03835 |
| 6348 | 0.03837 |
| 5248 | 0.03841 |
| 6648 | 0.03852 |
| 6248 | 0.03858 |
| 3.800 | 5648 | 0.03831 |
| 6548 | 0.03835 |
| 6348 | 0.03837 |
| 5248 | 0.03841 |
| 6648 | 0.03852 |
| 6248 | 0.03858 |
| Compound\_2 | 3.459 | 6348 | 0.03891 |
| 6548 | 0.03894 |
| 5248 | 0.03896 |
| 2648 | 0.03898 |
| 6648 | 0.03914 |
| 6248 | 0.03916 |
| 3.600 | 6348 | 0.03891 |
| 6548 | 0.03894 |
| 5248 | 0.03896 |
| 2648 | 0.03898 |
| 6648 | 0.03914 |
| 6248 | 0.03916 |
| 3.800 | 5248 | 0.03896 |
| 2648 | 0.03898 |
| 6648 | 0.03914 |
| 6248 | 0.03916 |
| 2258 | 0.04042 |
| 2265 | 0.04059 |
| Compound\_3 | 3.459 | 3648 | 0.04458 |
| 5248 | 0.04458 |
| 5648 | 0.04460 |
| 2648 | 0.04472 |
| 6248 | 0.04473 |
| 6648 | 0.04478 |
| 3.600 | 3648 | 0.04458 |
| 5248 | 0.04458 |
| 5648 | 0.04460 |
| 2648 | 0.04472 |
| 6248 | 0.04473 |
| 6648 | 0.04478 |
| 3.800 | 3648 | 0.04458 |
| 5248 | 0.04458 |
| 5648 | 0.04460 |
| 2648 | 0.04472 |
| 6248 | 0.04473 |
| 6648 | 0.04478 |
| Phosphonite | Compound\_1 | 3.459 | 6647 | 0.04151 |
| 5248 | 0.04152 |
| 5648 | 0.04158 |
| 6248 | 0.04160 |
| 6548 | 0.04163 |
| 6648 | 0.04183 |
| 3.600 | 6647 | 0.04151 |
| 5248 | 0.04152 |
| 5648 | 0.04158 |
| 6248 | 0.04160 |
| 6548 | 0.04163 |
| 6648 | 0.04183 |
| 3.800 | 6647 | 0.04151 |
| 5248 | 0.04152 |
| 5648 | 0.04158 |
| 6248 | 0.04160 |
| 6548 | 0.04163 |
| 6648 | 0.04183 |
| Compound\_2 | 3.459 | 5248 | 0.03637 |
| 6647 | 0.03648 |
| 6548 | 0.03651 |
| 5648 | 0.03653 |
| 6248 | 0.03653 |
| 6648 | 0.03683 |
| 3.600 | 5248 | 0.03637 |
| 6647 | 0.03648 |
| 6548 | 0.03651 |
| 5648 | 0.03653 |
| 6248 | 0.03653 |
| 6648 | 0.03682 |
| 3.800 | 5248 | 0.03637 |
| 6647 | 0.03648 |
| 6548 | 0.03651 |
| 5648 | 0.03653 |
| 6248 | 0.03653 |
| 6648 | 0.03682 |
| Compound\_3 | 3.459 | 5648 | 0.03523 |
| 6647 | 0.03523 |
| 5248 | 0.03527 |
| 6548 | 0.03530 |
| 6248 | 0.03544 |
| 6648 | 0.03559 |
| 3.600 | 5648 | 0.03522 |
| 6647 | 0.03523 |
| 5248 | 0.03527 |
| 6548 | 0.03530 |
| 6248 | 0.03544 |
| 6648 | 0.03559 |
| 3.800 | 5648 | 0.03522 |
| 6647 | 0.03523 |
| 5248 | 0.03527 |
| 6548 | 0.03530 |
| 6248 | 0.03544 |
| 6648 | 0.03559 |
| Phosphonodiamidite | Compound\_1 | 3.459 | 6348 | 0.04856 |
| 6647 | 0.04859 |
| 6448 | 0.04862 |
| 5648 | 0.04864 |
| 6548 | 0.04872 |
| 6648 | 0.04882 |
| 3.600 | 6348 | 0.04856 |
| 6647 | 0.04859 |
| 6448 | 0.04862 |
| 5648 | 0.04864 |
| 6548 | 0.04872 |
| 6648 | 0.04882 |
| 3.800 | 6348 | 0.04856 |
| 6647 | 0.04859 |
| 6448 | 0.04862 |
| 5648 | 0.04864 |
| 6548 | 0.04872 |
| 6648 | 0.04882 |
| Compound\_2 | 3.459 | 5647 | 0.04324 |
| 6448 | 0.04328 |
| 5648 | 0.04341 |
| 6647 | 0.04341 |
| 6548 | 0.04345 |
| 6648 | 0.04363 |
| 3.600 | 5647 | 0.04324 |
| 6448 | 0.04328 |
| 5648 | 0.04341 |
| 6647 | 0.04341 |
| 6548 | 0.04345 |
| 6648 | 0.04363 |
| 3.800 | 5647 | 0.04324 |
| 6448 | 0.04328 |
| 5648 | 0.04341 |
| 6647 | 0.04341 |
| 6548 | 0.04345 |
| 6648 | 0.04363 |
| Compound\_3 | 3.459 | 5647 | 0.03932 |
| 4648 | 0.03934 |
| 5548 | 0.03939 |
| 6548 | 0.03941 |
| 5648 | 0.03958 |
| 6648 | 0.03960 |
| 3.600 | 5647 | 0.03932 |
| 4648 | 0.03934 |
| 5548 | 0.03939 |
| 6548 | 0.03941 |
| 5648 | 0.03958 |
| 6648 | 0.03960 |
| 3.800 | 5647 | 0.03932 |
| 4648 | 0.03934 |
| 5548 | 0.03939 |
| 6548 | 0.03941 |
| 5648 | 0.03958 |
| 6648 | 0.03960 |
| Phosphoroamidate | Compound\_1 | 3.459 | 4248 | 0.03868 |
| 2248 | 0.03875 |
| 2648 | 0.03875 |
| 5248 | 0.03886 |
| 6648 | 0.03886 |
| 6248 | 0.03909 |
| 3.600 | 4248 | 0.03868 |
| 2248 | 0.03875 |
| 2648 | 0.03875 |
| 5248 | 0.03886 |
| 6648 | 0.03886 |
| 6248 | 0.03909 |
| 3.800 | 4248 | 0.03868 |
| 2248 | 0.03875 |
| 2648 | 0.03875 |
| 5248 | 0.03886 |
| 6648 | 0.03886 |
| 6248 | 0.03909 |
| Compound\_2 | 3.459 | 5648 | 0.04305 |
| 2248 | 0.04313 |
| 5248 | 0.04317 |
| 6648 | 0.04323 |
| 2648 | 0.04325 |
| 6248 | 0.04335 |
| 3.600 | 5648 | 0.04305 |
| 2248 | 0.04313 |
| 5248 | 0.04317 |
| 6648 | 0.04323 |
| 2648 | 0.04325 |
| 6248 | 0.04335 |
| Compound\_3 | 3.459 | 6348 | 0.03422 |
| 2248 | 0.03423 |
| 2648 | 0.03425 |
| 5248 | 0.03435 |
| 6648 | 0.03440 |
| 6248 | 0.03466 |
| 3.600 | 6348 | 0.03422 |
| 2248 | 0.03423 |
| 2648 | 0.03425 |
| 5248 | 0.03435 |
| 6648 | 0.03440 |
| 6248 | 0.03466 |
| 3.800 | 6348 | 0.03422 |
| 2248 | 0.03423 |
| 2648 | 0.03425 |
| 5248 | 0.03435 |
| 6648 | 0.03440 |
| 6248 | 0.03466 |
| Phosphorodiamidate | Compound\_1 | 3.459 | 2648 | 0.03467 |
| 4248 | 0.03469 |
| 5648 | 0.03474 |
| 5248 | 0.03489 |
| 6648 | 0.03494 |
| 6248 | 0.03510 |
| 3.600 | 2648 | 0.03467 |
| 4248 | 0.03469 |
| 5648 | 0.03474 |
| 5248 | 0.03489 |
| 6648 | 0.03494 |
| 6248 | 0.03510 |
| 3.800 | 2648 | 0.03467 |
| 4248 | 0.03469 |
| 5648 | 0.03474 |
| 5248 | 0.03489 |
| 6648 | 0.03494 |
| 6248 | 0.03510 |
| Compound\_2 | 3.459 | 4248 | 0.03902 |
| 2248 | 0.03908 |
| 2648 | 0.03913 |
| 5248 | 0.03920 |
| 6648 | 0.03921 |
| 6248 | 0.03941 |
| 3.600 | 4248 | 0.03902 |
| 2248 | 0.03908 |
| 2648 | 0.03913 |
| 5248 | 0.03920 |
| 6648 | 0.03921 |
| 6248 | 0.03941 |
| 3.800 | 4248 | 0.03902 |
| 2248 | 0.03908 |
| 2648 | 0.03913 |
| 5248 | 0.03920 |
| 6648 | 0.03921 |
| 6248 | 0.03941 |
| Compound\_3 | 3.459 | 3648 | 0.03965 |
| 5648 | 0.03972 |
| 2648 | 0.03977 |
| 5248 | 0.03977 |
| 6648 | 0.03988 |
| 6248 | 0.03993 |
| 3.600 | 3648 | 0.03965 |
| 5648 | 0.03972 |
| 2648 | 0.03977 |
| 5248 | 0.03977 |
| 6648 | 0.03988 |
| 6248 | 0.03993 |
| 3.800 | 3648 | 0.03965 |
| 5648 | 0.03972 |
| 2648 | 0.03977 |
| 5248 | 0.03977 |
| 6648 | 0.03988 |
| 6248 | 0.03993 |
| Phosphorodiamidtite | Compound\_1 | 3.459 | 6448 | 0.04746 |
| 5648 | 0.04747 |
| 6647 | 0.04749 |
| 6248 | 0.04752 |
| 6548 | 0.04757 |
| 6648 | 0.04773 |
| 3.600 | 6448 | 0.04746 |
| 5648 | 0.04747 |
| 6647 | 0.04749 |
| 6248 | 0.04752 |
| 6548 | 0.04757 |
| 6648 | 0.04773 |
| 3.800 | 6448 | 0.04746 |
| 5648 | 0.04747 |
| 6647 | 0.04749 |
| 6248 | 0.04752 |
| 6548 | 0.04757 |
| 6648 | 0.04773 |
| Compound\_2 | 3.459 | 5648 | 0.03749 |
| 6548 | 0.03756 |
| 6647 | 0.03756 |
| 5248 | 0.03758 |
| 6248 | 0.03774 |
| 6648 | 0.03782 |
| 3.600 | 5648 | 0.03749 |
| 6548 | 0.03756 |
| 6647 | 0.03756 |
| 5248 | 0.03758 |
| 6248 | 0.03774 |
| 6648 | 0.03782 |
| 3.800 | 5648 | 0.03749 |
| 6548 | 0.03756 |
| 6647 | 0.03756 |
| 5248 | 0.03758 |
| 6248 | 0.03774 |
| 6648 | 0.03782 |
| Compound\_3 | 3.459 | 6647 | 0.04280 |
| 6448 | 0.04282 |
| 6348 | 0.04285 |
| 6548 | 0.04292 |
| 6248 | 0.04298 |
| 6648 | 0.04308 |
| 3.600 | 6647 | 0.04281 |
| 6448 | 0.04282 |
| 6348 | 0.04285 |
| 6548 | 0.04291 |
| 6248 | 0.04298 |
| 6648 | 0.04307 |
| 3.800 | 6647 | 0.04280 |
| 6448 | 0.04282 |
| 6348 | 0.04285 |
| 6548 | 0.04292 |
| 6248 | 0.04298 |
| 6648 | 0.04307 |
| Phosphorotriamidate | Compound\_1 | 3.459 | 4648 | 0.04610 |
| 3648 | 0.04611 |
| 5648 | 0.04617 |
| 6248 | 0.04617 |
| 2648 | 0.04618 |
| 6648 | 0.04629 |
| 3.600 | 4648 | 0.04603 |
| 3648 | 0.04604 |
| 5648 | 0.04610 |
| 6248 | 0.04610 |
| 2648 | 0.04611 |
| 6648 | 0.04622 |
| 3.800 | 4648 | 0.04610 |
| 3648 | 0.04611 |
| 5648 | 0.04617 |
| 6248 | 0.04617 |
| 2648 | 0.04618 |
| 6648 | 0.04629 |
| Compound\_2 | 3.459 | 4648 | 0.04431 |
| 3648 | 0.04434 |
| 5648 | 0.04439 |
| 6248 | 0.04441 |
| 2648 | 0.04445 |
| 6648 | 0.04457 |
| 3.600 | 4648 | 0.04431 |
| 3648 | 0.04434 |
| 5648 | 0.04439 |
| 6248 | 0.04441 |
| 2648 | 0.04445 |
| 6648 | 0.04457 |
| 3.800 | 4648 | 0.04431 |
| 3648 | 0.04434 |
| 5648 | 0.04439 |
| 6248 | 0.04441 |
| 2648 | 0.04445 |
| 6648 | 0.04457 |
| Compound\_3 | 3.459 | 5248 | 0.04146 |
| 3648 | 0.04147 |
| 5648 | 0.04149 |
| 2648 | 0.04161 |
| 6248 | 0.04161 |
| 6648 | 0.04165 |
| 3.800 | 5248 | 0.04146 |
| 3648 | 0.04147 |
| 5648 | 0.04149 |
| 2648 | 0.04161 |
| 6248 | 0.04161 |
| 6648 | 0.04165 |
| Phosphorotriamidite | Compound\_1 | 3.459 | 6348 | 0.04041 |
| 6248 | 0.04042 |
| 6448 | 0.04050 |
| 6647 | 0.04053 |
| 6548 | 0.04065 |
| 6648 | 0.04081 |
| 3.600 | 6348 | 0.04041 |
| 6248 | 0.04042 |
| 6448 | 0.04050 |
| 6647 | 0.04053 |
| 6548 | 0.04065 |
| 6648 | 0.04081 |
| 3.800 | 6348 | 0.04041 |
| 6248 | 0.04042 |
| 6448 | 0.04050 |
| 6647 | 0.04053 |
| 6548 | 0.04065 |
| 6648 | 0.04081 |
| Compound\_2 | 3.459 | 5648 | 0.04795 |
| 6348 | 0.04795 |
| 6248 | 0.04796 |
| 6448 | 0.04800 |
| 6548 | 0.04807 |
| 6648 | 0.04814 |
| 3.600 | 5648 | 0.04795 |
| 6348 | 0.04795 |
| 6248 | 0.04796 |
| 6448 | 0.04800 |
| 6548 | 0.04807 |
| 6648 | 0.04814 |
| 3.800 | 5648 | 0.04795 |
| 6348 | 0.04795 |
| 6248 | 0.04796 |
| 6448 | 0.04800 |
| 6548 | 0.04807 |
| 6648 | 0.04814 |
| Compound\_3 | 3.459 | 5648 | 0.04433 |
| 6248 | 0.04441 |
| 6348 | 0.04441 |
| 6448 | 0.04445 |
| 6548 | 0.04451 |
| 6648 | 0.04457 |
| 3.600 | 5648 | 0.04433 |
| 6248 | 0.04441 |
| 6348 | 0.04441 |
| 6448 | 0.04445 |
| 6548 | 0.04451 |
| 6648 | 0.04457 |
| 3.800 | 5648 | 0.04433 |
| 6248 | 0.04441 |
| 6348 | 0.04441 |
| 6448 | 0.04445 |
| 6548 | 0.04451 |
| 6648 | 0.04457 |