**Supplemental file**

***In-silico* assay of a dosing vehicle based on chitosan-TiO2 and modified benzofuran-isatin molecules against *Pseudomonas aeruginosa***

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**S.1. Molecular docking data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Table S. Ligand Efficiency (kcal/mol), for LpxC protein: PDB 4J3D**  **Cavity: Volume 145.408 A3,** | | | | | |
| Name | Target | Target-NT | Target-QT | Target-NTQT | Target-QTNT |
| BRA | -4.710 | -4.891 | -4.591 | -5.357 | -3.342 |
| BRB | -4.876 | -4.912 | -4.657 | -4.543 | -3.264 |
| C-AZI | -2.570 | -2.512 | -2.966 | -2.279 | 0.988 |
| C-CIP | -4.166 | -3.954 | -3.587 | -4.250 | -2.522 |
| IRA | -5.172 | -5.169 | -4.140 | -4.894 | -2.857 |
| IRB | -4.838 | -4.836 | -4.100 | -4.866 | -2.851 |
| JS\_303 | -5.023 | -4.194 | -4.278 | -4.749 | -2.657 |
| MOL-A | -4.554 | -4.304 | -3.834 | -4.181 | -2.987 |
| MOL-B | -4.703 | -4.223 | -3.984 | -4.150 | -2.884 |
| MOL-C | -4.818 | -4.041 | -4.097 | -4.194 | -2.642 |
| MOL-D | -4.761 | -4.141 | -3.800 | -4.541 | -2.759 |
| MOL-E | -4.347 | -4.130 | -3.875 | -4.221 | -2.861 |
| MOL-F | -4.398 | -4.154 | -4.134 | -4.357 | -3.022 |
| MOL-G | -4.726 | -4.248 | -3.778 | -4.343 | -2.971 |
| MOL-H | -3.842 | -3.653 | -3.308 | -4.172 | -2.691 |
| MOL-I | -4.793 | -4.338 | -3.938 | -4.346 | -2.616 |
| MOL-J | -4.808 | -4.173 | -3.902 | -4.184 | -2.871 |
| NT | -4.222 | - | -4.292 | - | - |
| QT | -3.238 | -3.106 | - | - | - |

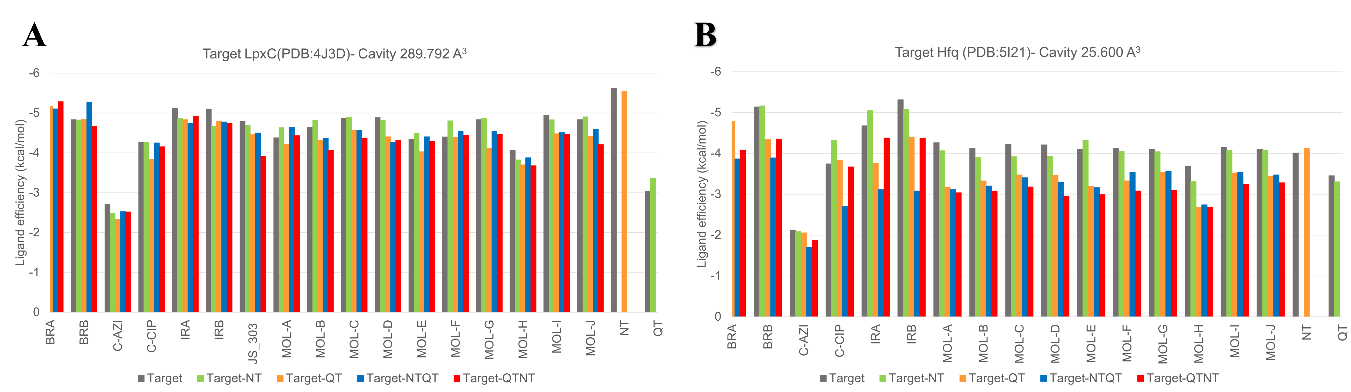


Figure S1 Ligand efficiency for a) LpxC, and b) Hfq.

**S.2. Cartesian coordinates of bioactive poses (Docking data)**

**Hfq**

Mol-A

C -2.87670 58.98100 -7.00880

C -3.74020 58.51310 -6.01590

C -1.59660 58.43510 -7.12210

C -1.16600 57.42700 -6.25970

C -2.04390 56.96200 -5.27300

C -3.31790 57.49910 -5.14750

O -5.03000 58.98030 -5.81010

C 0.24090 56.87080 -6.38620

N 0.88450 57.42400 -7.57830

C 1.42420 56.64390 -8.59360

H 0.67860 58.39690 -7.78270

C 2.58050 55.88510 -8.35050

C 3.10010 55.09280 -9.37460

C 2.45720 55.06350 -10.62660

C 1.32030 55.80480 -10.90100

C 0.81620 56.60000 -9.87770

C 4.24140 54.19960 -9.48460

C 4.22230 53.70300 -10.74420

O 3.14420 54.20120 -11.49380

C 5.13200 52.75580 -11.40660

N 4.78250 51.44140 -11.12390

O 6.07270 53.11000 -12.11410

N 5.54310 50.43410 -11.67240

H 3.97690 51.20800 -10.52290

C 5.03170 49.79800 -12.67700

C 5.65610 48.70050 -13.41170

C 4.75170 48.31240 -14.42260

N 3.59440 49.12470 -14.34210

C 3.69080 50.04420 -13.31150

O 2.85000 50.89590 -12.97770

H 2.78890 49.05920 -14.95200

C 6.87630 48.05960 -13.26930

C 5.05030 47.28440 -15.30140

C 7.18850 47.01880 -14.15200

C 6.28680 46.64090 -15.15070

H -3.18270 59.76280 -7.69110

H -0.92040 58.79300 -7.89060

H -1.72720 56.17120 -4.60140

H -4.01290 57.15430 -4.39370

H 0.82600 57.16900 -5.50590

H 0.20450 55.76990 -6.39950

C -6.12750 58.07510 -6.10700

H -7.03090 58.64070 -5.88490

H -6.08740 57.17840 -5.47840

H -6.12630 57.77840 -7.16170

H -0.05660 57.20750 -10.07370

H 0.85420 55.77170 -11.87580

H 3.05160 55.91160 -7.37520

H 4.97190 53.96100 -8.73090

H 4.35800 46.98620 -16.07800

H 6.54410 45.83410 -15.82580

H 8.13560 46.50250 -14.06170

H 7.55940 48.36860 -12.48780

**Hfq-NT**

MOL-E

C -3.66350 60.08890 -6.12350

C -5.01680 59.81090 -6.21680

C -2.76710 59.06890 -5.81000

C -3.22960 57.76870 -5.58630

C -4.59550 57.49990 -5.68890

C -5.47950 58.51860 -6.00130

C -2.24670 56.67360 -5.21010

N -1.32790 56.43730 -6.32110

C 0.05950 56.50090 -6.20310

H -1.70750 55.91960 -7.10830

C 0.66430 57.70920 -5.82400

C 2.05170 57.75930 -5.68670

C 2.81620 56.60070 -5.92170

C 2.25080 55.39650 -6.30580

C 0.86810 55.36070 -6.45350

C 2.99590 58.80040 -5.31870

C 4.22510 58.23420 -5.35040

O 4.17510 56.87900 -5.71590

C 5.54540 58.81630 -5.06220

N 5.99580 59.59380 -6.12010

O 6.14900 58.61790 -4.00980

N 7.22450 60.20420 -5.99990

H 5.44130 59.72060 -6.98060

C 7.22480 61.45220 -5.65760

C 8.40310 62.29550 -5.47150

C 7.94050 63.57650 -5.10350

N 6.52520 63.55930 -5.05470

C 6.02170 62.31080 -5.37740

O 4.82920 61.96600 -5.42680

H 5.93760 64.34840 -4.81520

C 9.75970 62.04070 -5.59250

C 8.82010 64.61640 -4.85320

C 10.65820 63.08470 -5.34140

C 10.19110 64.35060 -4.97790

H -3.32850 61.10260 -6.29660

H -1.70560 59.26990 -5.73770

F -6.81900 58.25980 -6.11060

H -1.66280 57.01190 -4.34470

H -2.79490 55.76840 -4.90530

H 0.40600 54.43890 -6.77960

H 2.86410 54.52610 -6.49290

H 0.05520 58.58460 -5.63220

H 2.78790 59.82560 -5.06430

H 8.46660 65.59960 -4.57050

H 10.89970 65.14720 -4.78710

H 11.72290 62.91060 -5.42860

H 10.09940 61.05220 -5.87620

F -5.91120 60.79950 -6.52520

H -4.98710 56.50240 -5.53390

**LpxC**

MOL-I

C -0.89570 -7.82780 -14.75360

C -1.77900 -8.04650 -13.69620

C -0.35370 -8.90410 -15.45420

C -0.69070 -10.21500 -15.09720

C -1.57550 -10.43790 -14.04330

C -2.10400 -9.35160 -13.35880

C -0.07140 -11.38000 -15.85060

N -1.10960 -12.08570 -16.59870

C -1.95230 -11.47140 -17.51990

H -1.01880 -13.09610 -16.64180

C -3.29220 -11.22950 -17.17840

C -4.12350 -10.59510 -18.10160

C -3.60560 -10.20400 -19.35090

C -2.29170 -10.43560 -19.72150

C -1.47400 -11.08010 -18.79910

C -5.51890 -10.19020 -18.09660

C -5.75390 -9.60230 -19.29310

O -4.60990 -9.58230 -20.10780

C -6.98610 -9.00490 -19.83080

N -7.49260 -9.75560 -20.88330

O -7.47920 -7.97060 -19.38580

N -8.64700 -9.32010 -21.49460

H -7.02990 -10.61710 -21.21180

C -8.77310 -9.57860 -22.75640

C -9.90710 -9.21410 -23.60240

C -9.62430 -9.68990 -24.89990

N -8.36270 -10.33330 -24.89050

C -7.78880 -10.30580 -23.63110

O -6.69260 -10.77970 -23.28940

H -7.91940 -10.76530 -25.69190

C -11.08920 -8.54150 -23.33740

C -10.51150 -9.50200 -25.94640

C -11.99400 -8.34610 -24.38780

C -11.70540 -8.82060 -25.67010

H 0.66290 -10.98350 -16.56380

H 0.46870 -12.03430 -15.14880

H -0.45090 -11.29580 -19.07510

H -1.92440 -10.13570 -20.69300

H -3.66640 -11.52560 -16.20550

H -6.24410 -10.31770 -17.31130

H -10.29610 -9.86690 -26.94230

H -12.41630 -8.66100 -26.47160

H -12.92470 -7.82430 -24.20590

H -11.29210 -8.18180 -22.33630

H -0.63150 -6.81440 -15.02910

H 0.33000 -8.74460 -16.27920

F -2.97980 -9.58040 -12.32700

H -1.86380 -11.43970 -13.75090

H -2.21550 -7.22910 -13.13890

**LpxC-NT**

MOL-J

C -2.38000 -10.17990 -12.81200

C -2.45020 -8.79250 -12.96110

C -1.60830 -10.93840 -13.68990

C -0.90160 -10.31710 -14.72610

C -0.97070 -8.93040 -14.86890

C -1.74490 -8.16940 -13.99030

C -0.08520 -11.16630 -15.68580

N -0.98400 -11.89330 -16.58180

C -1.83900 -11.27730 -17.48720

H -0.77830 -12.87840 -16.71610

C -3.20040 -11.13720 -17.17310

C -4.04450 -10.49930 -18.08230

C -3.51930 -10.00400 -19.29090

C -2.18410 -10.13310 -19.63440

C -1.35250 -10.78050 -18.72680

C -5.46170 -10.17890 -18.09500

C -5.70110 -9.53530 -19.26160

O -4.53990 -9.39890 -20.03990

C -6.95240 -8.98040 -19.79970

N -7.43460 -9.74960 -20.85100

O -7.48040 -7.96250 -19.35690

N -8.60090 -9.35110 -21.46370

H -6.94440 -10.59670 -21.17650

C -8.72470 -9.62430 -22.72240

C -9.86990 -9.29420 -23.56760

C -9.57940 -9.77310 -24.86260

N -8.30320 -10.38650 -24.85170

C -7.72630 -10.33490 -23.59400

O -6.61810 -10.78000 -23.25230

H -7.85120 -10.81280 -25.65110

C -11.06670 -8.64770 -23.30430

C -10.47400 -9.61380 -25.90770

C -11.97870 -8.48140 -24.35340

C -11.68250 -8.95840 -25.63320

H 0.55000 -10.50560 -16.29060

H 0.57990 -11.83600 -15.11860

H -0.31020 -10.91500 -18.98160

H -1.81060 -9.75320 -20.57510

H -3.58110 -11.51350 -16.23100

H -6.19760 -10.39570 -17.33990

H -10.25220 -9.98080 -26.90160

H -12.39900 -8.82130 -26.43360

H -12.92060 -7.97970 -24.17270

H -11.27540 -8.28540 -22.30520

H -3.04880 -8.20220 -12.27790

H -2.92620 -10.66760 -12.01350

H -1.54260 -12.01550 -13.58330

H -0.41580 -8.44460 -15.66440

H -1.79090 -7.09320 -14.10650

**S.3. DFT and reactivity index data**

Mol-A

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | Cation | Anion | | Neutro |
| Atom | No | Charge | No | Charge | Charge |
| C | 1.0000 | -0.1438 |  | -0.2930 | -0.2928 |
| C | 2.0000 | 0.1677 |  | 0.3233 | 0.3238 |
| C | 3.0000 | -0.0944 |  | -0.1930 | -0.1929 |
| C | 4.0000 | -0.0469 |  | -0.0811 | -0.0817 |
| C | 5.0000 | -0.0924 |  | -0.1938 | -0.1935 |
| C | 6.0000 | -0.1226 |  | -0.2541 | -0.2538 |
| O | 7.0000 | -0.2881 |  | -0.5816 | -0.5814 |
| C | 8.0000 | -0.1257 |  | -0.1916 | -0.1921 |
| N | 9.0000 | 0.0584 |  | -0.6638 | -0.6614 |
| C | 10.0000 | 0.1070 |  | 0.1776 | 0.1793 |
| H | 11.0000 | 0.2150 |  | 0.4013 | 0.4029 |
| C | 12.0000 | 0.0658 |  | -0.2402 | -0.2294 |
| C | 13.0000 | -0.0919 |  | -0.1105 | -0.1170 |
| C | 14.0000 | 0.3035 |  | 0.2826 | 0.2927 |
| C | 15.0000 | -0.1270 |  | -0.2371 | -0.2348 |
| C | 16.0000 | -0.0162 |  | -0.2692 | -0.2526 |
| C | 17.0000 | -0.0812 |  | -0.2627 | -0.2103 |
| C | 18.0000 | 0.1077 |  | 0.2378 | 0.2160 |
| O | 19.0000 | -0.2287 |  | -0.5280 | -0.5224 |
| C | 20.0000 | 0.3298 |  | 0.6066 | 0.6604 |
| N | 21.0000 | -0.2341 |  | -0.4639 | -0.4723 |
| O | 22.0000 | -0.3117 |  | -0.7091 | -0.6348 |
| N | 23.0000 | -0.0938 |  | -0.3758 | -0.1855 |
| H | 24.0000 | 0.2284 |  | 0.4483 | 0.4574 |
| C | 25.0000 | 0.0731 |  | 0.0012 | 0.1368 |
| C | 26.0000 | -0.0686 |  | -0.1197 | -0.1347 |
| C | 27.0000 | 0.0970 |  | 0.1636 | 0.1921 |
| N | 28.0000 | -0.3087 |  | -0.6380 | -0.6183 |
| C | 29.0000 | 0.3371 |  | 0.5932 | 0.6737 |
| O | 30.0000 | -0.3271 |  | -0.7672 | -0.6566 |
| H | 31.0000 | 0.2227 |  | 0.4242 | 0.4446 |
| C | 32.0000 | -0.0800 |  | -0.2262 | -0.1630 |
| C | 33.0000 | -0.1239 |  | -0.2565 | -0.2482 |
| C | 34.0000 | -0.1171 |  | -0.2464 | -0.2344 |
| C | 35.0000 | -0.0874 |  | -0.2492 | -0.1781 |
| H | 36.0000 | 0.1185 |  | 0.2319 | 0.2321 |
| H | 37.0000 | 0.1139 |  | 0.2287 | 0.2286 |
| H | 38.0000 | 0.1147 |  | 0.2243 | 0.2245 |
| H | 39.0000 | 0.1181 |  | 0.2313 | 0.2315 |
| H | 40.0000 | 0.1322 |  | 0.2109 | 0.2114 |
| H | 41.0000 | 0.1427 |  | 0.1958 | 0.1970 |
| C | 42.0000 | -0.1086 |  | -0.2165 | -0.2165 |
| H | 43.0000 | 0.1010 |  | 0.2002 | 0.2003 |
| H | 44.0000 | 0.0917 |  | 0.1820 | 0.1820 |
| H | 45.0000 | 0.0917 |  | 0.1820 | 0.1820 |
| H | 46.0000 | 0.1229 |  | 0.2269 | 0.2298 |
| H | 47.0000 | 0.1336 |  | 0.2385 | 0.2418 |
| H | 48.0000 | 0.1238 |  | 0.2266 | 0.2300 |
| H | 49.0000 | 0.1354 |  | 0.2512 | 0.2568 |
| H | 50.0000 | 0.1201 |  | 0.2259 | 0.2396 |
| H | 51.0000 | 0.1143 |  | 0.2155 | 0.2280 |
| H | 52.0000 | 0.1142 |  | 0.2150 | 0.2277 |
| H | 53.0000 | 0.1180 |  | 0.2218 | 0.2354 |

Mol-B

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | Cation | QT-Anion | QT-Neutro |
| Atom | No | Charge | Charge | Charge |
| C | 1 | -0.10534 | -0.21758 | -0.21735 |
| C | 2 | -0.09352 | -0.20131 | -0.20079 |
| C | 3 | -0.09688 | -0.19762 | -0.19751 |
| C | 4 | -0.05991 | -0.10768 | -0.10824 |
| C | 5 | 0.21055 | 0.41263 | 0.41297 |
| C | 6 | -0.13276 | -0.27302 | -0.27276 |
| C | 7 | -0.12698 | -0.19739 | -0.19779 |
| N | 8 | 0.05091 | -0.66464 | -0.66234 |
| C | 9 | 0.11799 | 0.18198 | 0.18364 |
| H | 10 | 0.21542 | 0.40091 | 0.40248 |
| C | 11 | 0.05871 | -0.25005 | -0.2389 |
| C | 12 | -0.08782 | -0.10485 | -0.1115 |
| C | 13 | 0.30619 | 0.28435 | 0.29439 |
| C | 14 | -0.12444 | -0.23658 | -0.2342 |
| C | 15 | -0.01853 | -0.26854 | -0.25196 |
| C | 16 | -0.08118 | -0.26221 | -0.20974 |
| C | 17 | 0.10412 | 0.23033 | 0.20851 |
| O | 18 | -0.22779 | -0.52812 | -0.52253 |
| C | 19 | 0.33537 | 0.61721 | 0.67106 |
| N | 20 | -0.23612 | -0.46809 | -0.47652 |
| O | 21 | -0.3105 | -0.7071 | -0.63251 |
| N | 22 | -0.09404 | -0.37588 | -0.18587 |
| H | 23 | 0.22839 | 0.44821 | 0.45737 |
| C | 24 | 0.07342 | 0.00157 | 0.13721 |
| C | 25 | -0.06863 | -0.11986 | -0.13477 |
| C | 26 | 0.09701 | 0.16366 | 0.19215 |
| N | 27 | -0.30865 | -0.63791 | -0.61817 |
| C | 28 | 0.3371 | 0.59356 | 0.67374 |
| O | 29 | -0.32694 | -0.76696 | -0.65634 |
| H | 30 | 0.22272 | 0.42417 | 0.44459 |
| C | 31 | -0.07985 | -0.22611 | -0.16281 |
| C | 32 | -0.12391 | -0.25643 | -0.24816 |
| C | 33 | -0.11705 | -0.24631 | -0.23432 |
| C | 34 | -0.08732 | -0.24919 | -0.17791 |
| H | 35 | 0.11591 | 0.22627 | 0.22645 |
| H | 36 | 0.11623 | 0.23399 | 0.23396 |
| F | 37 | -0.185 | -0.37538 | -0.37522 |
| H | 38 | 0.1227 | 0.24036 | 0.24057 |
| H | 39 | 0.13295 | 0.21973 | 0.22021 |
| H | 40 | 0.14693 | 0.20784 | 0.209 |
| H | 41 | 0.12329 | 0.22702 | 0.22996 |
| H | 42 | 0.13393 | 0.23895 | 0.24225 |
| H | 43 | 0.12492 | 0.2284 | 0.23178 |
| H | 44 | 0.13558 | 0.25128 | 0.25695 |
| H | 45 | 0.12013 | 0.22592 | 0.2396 |
| H | 46 | 0.11431 | 0.21557 | 0.22803 |
| H | 47 | 0.11418 | 0.21502 | 0.22774 |
| H | 48 | 0.11794 | 0.2218 | 0.23533 |
| H | 49 | 0.11628 | 0.22813 | 0.22832 |

Mol-C

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | Cation | Anion | Neutro |
| Atom | No | Charge | Charge | Charge |
| C | 1 | -0.0976 | -0.20168 | -0.20147 |
| C | 2 | -0.09458 | -0.20352 | -0.20302 |
| C | 3 | -0.09773 | -0.20101 | -0.20093 |
| C | 4 | -0.04218 | -0.07468 | -0.07518 |
| C | 5 | -0.04926 | -0.1039 | -0.10367 |
| C | 6 | -0.11199 | -0.23116 | -0.23091 |
| C | 7 | -0.12605 | -0.19759 | -0.19793 |
| N | 8 | 0.0471 | -0.66502 | -0.66271 |
| C | 9 | 0.11964 | 0.1825 | 0.18418 |
| H | 10 | 0.21444 | 0.40021 | 0.4018 |
| C | 11 | 0.05842 | -0.25037 | -0.23919 |
| C | 12 | -0.08715 | -0.10408 | -0.11073 |
| C | 13 | 0.30571 | 0.28361 | 0.29359 |
| C | 14 | -0.12392 | -0.23611 | -0.23371 |
| C | 15 | -0.01902 | -0.26817 | -0.25152 |
| C | 16 | -0.08101 | -0.26252 | -0.20995 |
| C | 17 | 0.10382 | 0.22971 | 0.20796 |
| O | 18 | -0.22621 | -0.52567 | -0.51996 |
| C | 19 | 0.33516 | 0.6169 | 0.67066 |
| N | 20 | -0.23592 | -0.46769 | -0.47616 |
| O | 21 | -0.31001 | -0.70592 | -0.63151 |
| N | 22 | -0.09436 | -0.376 | -0.1865 |
| H | 23 | 0.22825 | 0.44775 | 0.45703 |
| C | 24 | 0.07356 | 0.0026 | 0.13752 |
| C | 25 | -0.06845 | -0.11996 | -0.13442 |
| C | 26 | 0.09671 | 0.16305 | 0.19154 |
| N | 27 | -0.30867 | -0.63739 | -0.61819 |
| C | 28 | 0.33724 | 0.59361 | 0.67401 |
| O | 29 | -0.32636 | -0.76576 | -0.65517 |
| H | 30 | 0.22293 | 0.42457 | 0.44502 |
| C | 31 | -0.08 | -0.2267 | -0.16309 |
| C | 32 | -0.12389 | -0.2563 | -0.2481 |
| C | 33 | -0.11709 | -0.24642 | -0.23441 |
| C | 34 | -0.08739 | -0.24979 | -0.17805 |
| H | 35 | 0.13206 | 0.22311 | 0.22348 |
| H | 36 | 0.14729 | 0.20975 | 0.21089 |
| H | 37 | 0.12296 | 0.22623 | 0.22917 |
| H | 38 | 0.13369 | 0.23852 | 0.24182 |
| H | 39 | 0.12466 | 0.22779 | 0.23118 |
| H | 40 | 0.13554 | 0.25116 | 0.25685 |
| H | 41 | 0.1198 | 0.22526 | 0.23896 |
| H | 42 | 0.11428 | 0.21547 | 0.22797 |
| H | 43 | 0.1141 | 0.21481 | 0.22759 |
| H | 44 | 0.11792 | 0.22174 | 0.23529 |
| H | 45 | 0.11699 | 0.22952 | 0.2297 |
| H | 46 | 0.11621 | 0.22665 | 0.22682 |
| H | 47 | 0.1157 | 0.23688 | 0.23675 |
| Br | 48 | 0.03402 | 0.04938 | 0.04985 |
| H | 49 | 0.1207 | 0.2367 | 0.2369 |

Mol-D

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | Cation | Anion | Neutro |
| Atom | No | Charge | Charge | Charge |
| C | 1 | -0.09876 | -0.20402 | -0.20381 |
| C | 2 | -0.0939 | -0.20208 | -0.20158 |
| C | 3 | -0.09728 | -0.20098 | -0.20088 |
| C | 4 | -0.04214 | -0.07683 | -0.0773 |
| C | 5 | -0.00353 | -0.0112 | -0.01097 |
| C | 6 | -0.11481 | -0.23683 | -0.23657 |
| C | 7 | -0.12584 | -0.19677 | -0.19708 |
| N | 8 | 0.04713 | -0.66988 | -0.66767 |
| C | 9 | 0.12001 | 0.17652 | 0.17825 |
| H | 10 | 0.21485 | 0.39994 | 0.40154 |
| C | 11 | 0.0623 | -0.23548 | -0.22434 |
| C | 12 | -0.08928 | -0.11036 | -0.11689 |
| C | 13 | 0.30591 | 0.28661 | 0.29656 |
| C | 14 | -0.12269 | -0.23688 | -0.23447 |
| C | 15 | -0.02044 | -0.26583 | -0.24938 |
| C | 16 | -0.08163 | -0.26226 | -0.20983 |
| C | 17 | 0.10457 | 0.23039 | 0.2087 |
| O | 18 | -0.22728 | -0.5277 | -0.52216 |
| C | 19 | 0.33539 | 0.61736 | 0.67117 |
| N | 20 | -0.23612 | -0.46808 | -0.47663 |
| O | 21 | -0.31041 | -0.70698 | -0.63239 |
| N | 22 | -0.09417 | -0.37608 | -0.18612 |
| H | 23 | 0.22839 | 0.44824 | 0.45739 |
| C | 24 | 0.07372 | 0.00191 | 0.13779 |
| C | 25 | -0.06864 | -0.11992 | -0.1348 |
| C | 26 | 0.09702 | 0.1636 | 0.19215 |
| N | 27 | -0.30861 | -0.63782 | -0.61809 |
| C | 28 | 0.33712 | 0.59363 | 0.67377 |
| O | 29 | -0.32692 | -0.76688 | -0.65629 |
| H | 30 | 0.22273 | 0.42422 | 0.44462 |
| C | 31 | -0.07979 | -0.22609 | -0.16269 |
| C | 32 | -0.12393 | -0.2564 | -0.24818 |
| C | 33 | -0.11705 | -0.24628 | -0.23431 |
| C | 34 | -0.08725 | -0.24914 | -0.17778 |
| H | 35 | 0.11645 | 0.22702 | 0.22719 |
| H | 36 | 0.11562 | 0.23736 | 0.23723 |
| Cl | 37 | -0.01446 | -0.04507 | -0.04468 |
| H | 38 | 0.1228 | 0.24077 | 0.24097 |
| H | 39 | 0.13129 | 0.2251 | 0.22542 |
| H | 40 | 0.14821 | 0.21012 | 0.21125 |
| H | 41 | 0.12341 | 0.22678 | 0.22972 |
| H | 42 | 0.13406 | 0.23919 | 0.24248 |
| H | 43 | 0.12466 | 0.22765 | 0.23104 |
| H | 44 | 0.13569 | 0.25151 | 0.25718 |
| H | 45 | 0.12013 | 0.22594 | 0.2396 |
| H | 46 | 0.11433 | 0.21561 | 0.22807 |
| H | 47 | 0.1142 | 0.21505 | 0.22777 |
| H | 48 | 0.11798 | 0.22185 | 0.2354 |
| H | 49 | 0.11702 | 0.22954 | 0.22973 |

Mol-E

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | Cation | Anion | Neutro |
| Atom | No | Charge | Charge | Charge |
| C | 1 | -0.24575 | -0.25273 | -0.2525 |
| C | 2 | 0.35999 | 0.34748 | 0.34794 |
| C | 3 | -0.20188 | -0.20416 | -0.20404 |
| C | 4 | -0.05452 | -0.03729 | -0.03784 |
| C | 5 | -0.24824 | -0.25941 | -0.25902 |
| C | 6 | 0.36612 | 0.3603 | 0.36051 |
| C | 7 | -0.23039 | -0.19419 | -0.19457 |
| N | 8 | -0.37449 | -0.66513 | -0.66288 |
| C | 9 | 0.19575 | 0.18161 | 0.18327 |
| H | 10 | 0.44354 | 0.40165 | 0.40322 |
| C | 11 | -0.09919 | -0.24965 | -0.23851 |
| C | 12 | -0.11905 | -0.1046 | -0.11123 |
| C | 13 | 0.41598 | 0.28454 | 0.29449 |
| C | 14 | -0.20942 | -0.23634 | -0.23396 |
| C | 15 | -0.16661 | -0.26837 | -0.25188 |
| C | 16 | -0.19238 | -0.26235 | -0.21008 |
| C | 17 | 0.23458 | 0.23065 | 0.2089 |
| O | 18 | -0.49035 | -0.52791 | -0.52235 |
| C | 19 | 0.66938 | 0.61739 | 0.67106 |
| N | 20 | -0.47286 | -0.46818 | -0.47657 |
| O | 21 | -0.61523 | -0.70704 | -0.63257 |
| N | 22 | -0.188 | -0.37612 | -0.18602 |
| H | 23 | 0.45684 | 0.44828 | 0.45742 |
| C | 24 | 0.14679 | 0.00175 | 0.13757 |
| C | 25 | -0.1372 | -0.11991 | -0.13478 |
| C | 26 | 0.19393 | 0.16367 | 0.19218 |
| N | 27 | -0.61719 | -0.63788 | -0.61811 |
| C | 28 | 0.67427 | 0.59352 | 0.67378 |
| O | 29 | -0.65417 | -0.76714 | -0.65646 |
| H | 30 | 0.44551 | 0.42422 | 0.44466 |
| C | 31 | -0.15979 | -0.22607 | -0.16274 |
| C | 32 | -0.2477 | -0.25636 | -0.24809 |
| C | 33 | -0.23398 | -0.24624 | -0.23425 |
| C | 34 | -0.17473 | -0.24913 | -0.17782 |
| H | 35 | 0.25217 | 0.24656 | 0.24674 |
| H | 36 | 0.2385 | 0.23922 | 0.23917 |
| F | 37 | -0.35228 | -0.35735 | -0.35715 |
| H | 38 | 0.25164 | 0.21911 | 0.21956 |
| H | 39 | 0.25768 | 0.20025 | 0.20148 |
| H | 40 | 0.25182 | 0.22703 | 0.22996 |
| H | 41 | 0.26733 | 0.23905 | 0.24234 |
| H | 42 | 0.25813 | 0.22853 | 0.2319 |
| H | 43 | 0.27241 | 0.25144 | 0.2571 |
| H | 44 | 0.24029 | 0.22594 | 0.23965 |
| H | 45 | 0.22862 | 0.21555 | 0.22803 |
| H | 46 | 0.22836 | 0.215 | 0.22774 |
| H | 47 | 0.23592 | 0.22181 | 0.23536 |
| F | 48 | -0.35285 | -0.35809 | -0.35788 |
| H | 49 | 0.25275 | 0.24715 | 0.24734 |