**Supplementary Information**

**Title: Chemical Reactivity Theory (CRT) Study of Small Drug-like biologically active Molecules**

**Submitted by:**

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**Theoretical Background:**

Molecular Descriptors are used to predict the quantitative reactivity of the molecular system.Various formulas are used to calculate the global and local reactivity descriptors which are given below:

1. Electronegativity
2. Global Hardness *η* = (I – A)
3. Electrophilicity *ω =*

(4) Electron-donating Power

(5) Electron-accepting Power

(6) Net Electrophilicity =

(7) The maximal amount of electronic charge that an electrophile may accept, Qmax,

Qmax=

(8) Dual Descriptor

where , represents the electron densities at “r” for system with N + 1, N, and N − 1 electrons, respectively and represents the atomic spin density (ASD) at the “r” atom of the radical anion or cation of a given molecule, respectively.

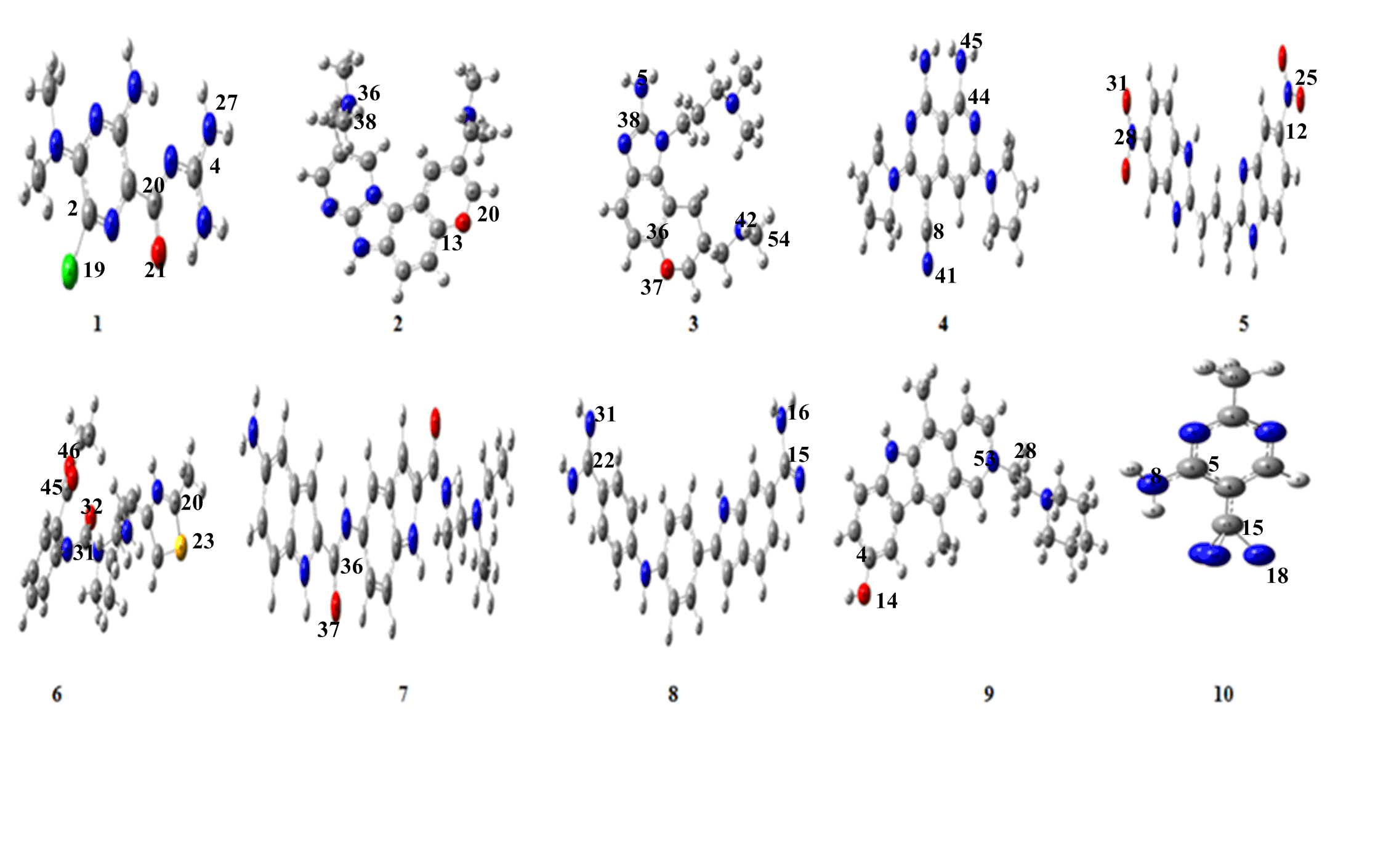
Fukui function has the ability of the molecular site to accept or donate electrons. It is defined as the derivative of ρ(**r**) with respect to *N.* f +(**r**), is related to the reactivity for a nucleophilic attack and f −(**r**) is related to the reactivity for an electrophilic attack. The condensed Fukui function based on the Natural Bond Orbital (NBO) theory was calculated by:

(9)

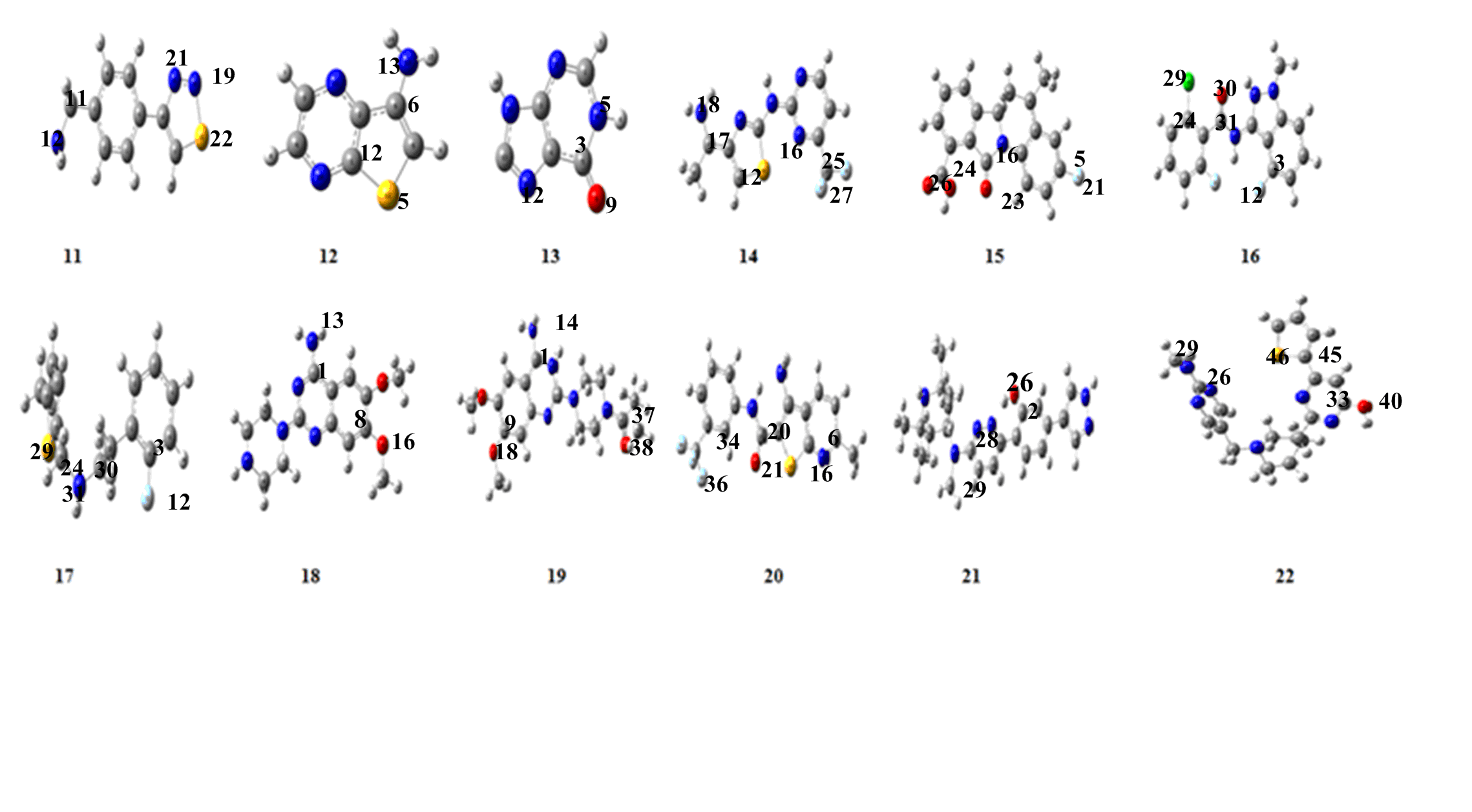
(10)

(11) The nucleophilicity N*1* index

N*1*=

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**Supplementary Figure 1(a):** Optimized Structures for complexes **1-10**. Atom numbering for Bondlengths is given here. Color code for atoms is mentioned here. Blue: N, Red: O, Yellow: S, Gray: C, Green: Cl.

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**Supplementary Figure 1(b):** Optimized Structures for complexes **11-22**. Atom numbering for Bondlengths is given here. Color code for atoms is mentioned here. Blue: N, Red: O, Yellow: S, Gray: C, Green: Cl.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** |  | **Bondlengths(Å)** | | |  |  | **Bondlengths(Å)** | | |
|  |  | B3LYP/6-31G\*\* | MP2/6-31G\*\* | M05-2x/6-31G\*\* |  |  | B3LYP/6-31G\*\* | MP2/6-31G\*\* | M05-2x/6-31G\*\* |
| **1** | C2-Cl19 | 1.7633 | 1.7922 | 1.7692 | **12** | C12-S5 | 1.7394 | 1.750 | 1.7351 |
|  | C20=O21 | 1.2319 | 1.2438 | 1.2317 |  | C6-N13 | 1.3794 | 1.3861 | 1.3761 |
|  | C4-N27 | 1.3458 | 1.3399 | 1.3455 | **13** | C5=O9 | 1.2107 | 1.2097 | 1.2097 |
| **2** | C13-O20 | 1.3602 | 1.3608 | 1.3681 |  | C3-N12 | 1.3532 | 1.3531 | 1.3544 |
|  | C38-N36 | 1.4521 | 1.4517 | 1.4506 | **14** | C12-S16 | 1.7503 | 1.7668 | 1.7568 |
| **3** | C36-O37 | 1.4459 | 1.4461 | 1.4458 |  | C25-F27 | 1.3318 | 1.3459 | 1.3459 |
|  | N5-C38 | 1.4577 | 1.4579 | 1.4576 |  | C17-N18 | 1.3853 | 1.3868 | 1.3868 |
|  | N42-C54 | 1.4782 | 1.4785 | 1.4785 | **15** | C16=O23 | 1.2144 | 1.2126 | 1.2126 |
| **4** | C44-N45 | 1.3944 | 1.3946 | 1.3944 |  | C5-F21 | 1.3394 | 1.3543 | 1.3344 |
|  | C8-N41 | 1.3587 | 1.3594 | 1.3592 |  | C24=026 | 1.3418 | 1.3434 | 1.3455 |
| **5** | C12-N25 | 1.4766 | 1.4769 | 1.4768 | **16** | C24-Cl29 | 1.7427 | 1.7519 | 1.7419 |
|  | N28-O31 | 1.2248 | 1.2249 | 1.2247 |  | C30=O31 | 1.2274 | 1.2316 | 1.2214 |
| **6** | C20-S23 | 1.7687 | 1.8004 | 1.7682 |  | C3-F12 | 1.3459 | 1.3621 | 1.3421 |
|  | C31-O32 | 1.4444 | 1.3485 | 1.4468 | **17** | C24-S29 | 1.7394 | 1.7526 | 1.7526 |
|  | C45=O46 | 1.2179 | 1.2067 | 1.2173 |  | C30-N31 | 1.4599 | 1.4645 | 1.4601 |
| **7** | C36=O37 | 1.2264 | 1.2332 | 1.2232 |  | C3-F12 | 1.3435 | 1.3591 | 1.3590 |
|  | C5-N38 | 1.3968 | 1.4041 | 1.4042 | **18** | C1-N13 | 1.3998 | 1.3706 | 1.4064 |
|  | N42-C54 | 1.4586 | 1.4701 | 1.4511 |  | C8-O16 | 1.3612 | 1.3592 | 1.3609 |
| **8** | C15-N16 | 1.3841 | 1.3945 | 1.3809 | **19** | C37=O38 | 1.2208 | 1.2226 | 1.2206 |
|  | C22-N31 | 1.3907 | 1.3906 | 1.3904 |  | C1-N14 | 1.3981 | 1.4048 | 1.4001 |
| **9** | C4=O14 | 1.3646 | 1.3761 | 1.3661 |  | C9-O18 | 1.3594 | 1.3744 | 1.3583 |
|  | N53-C28 | 1.4582 | 1.4663 | 1.4565 | **20** | C6-S16 | 1.7176 | 1.7567 | 1.7174 |
|  | N-C2H5 | 1.4687 | 1.4663 | 1.4663 |  | C20=O21 | 1.2251 | 1.2216 | 1.2215 |
| **10** | C5-N8 | 1.3512 | 1.3553 | 1.3553 |  | C34-F36 | 1.3412 | 1.3483 | 1.3482 |
|  | C15=N18 | 1.4221 | 1.4236 | 1.4235 | **21** | N28-C29 | 1.4624 | 1.4719 | 1.4717 |
| **11** | N19-S22 | 1.7273 | 1.7556 | 1.7256 |  | N2-O26 | 1.3328 | 1.3405 | 1.3402 |
|  | N19-N21 | 1.2675 | 1.2628 | 1.2628 | **22** | C45-S46 | 1.7357 | 1.7468 | 1.7468 |
|  | C11-N12 | 1.4471 | 1.4571 | 1.4570 |  | N26-C29 | 1.4394 | 1.4492 | 1.4493 |
|  |  |  |  |  |  | C33=O40 | 1.3369 | 1.3445 | 1.3444 |
|  |  |  |  |  |  |  |  |  |  |

**Supplementary Table 1:** Geometrical parameters (Bond lengths) of **1-22** complexes with **(a)** B3LYP/6-31G\*\*, **(b)** MP2/6-31G\*\* and **(c)** M05-2x/6-31G\*\* DFT method. Water is used as a solvent.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **1** | | **2** | | **3** | | **4** | | **5** | | **6** | |
|  |  |  |  |  |  |  |  |  |  |  |  |
| 1 | 0.0291 | 0.0558 | -0.0224 | 0.0408 | -0.1376 | -0.1098 | 0.0751 | 0.2326 | 0.0358 | -0.0856 | -0.1222 | 0.0959 |
| 2 | 0.1727 | -0.0985 | 0.0370 | -0.0319 | 0.0340 | 0.1146 | -0.0548 | 0.0583 | 0.2794 | 0.3794 | -0.1210 | 0.0903 |
| 3 | 0.1002 | 0.0051 | 0.0499 | 0.0519 | -0.0433 | 0.0278 | -0.2238 | -0.0355 | -0.2197 | -0.1752 | -0.0905 | 0.0891 |
| 4 | 0.0814 | -0.0160 | 0.1658 | -0.1477 | -0.1704 | -0.1134 | -0.0723 | -0.0843 | -0.6798 | -1.1884 | -0.1115 | 0.1100 |
| 5 | -0.0828 | 0.1694 | -0.1241 | 0.1831 | 0.1152 | 0.1718 | 0.0896 | 0.1085 | -0.4322 | -0.6012 | -0.1415 | 0.1394 |
| 6 | -0.1142 | 0.1783 | -0.1035 | 0.2040 | 0.0923 | 0.2215 | 0.0567 | 0.2527 | 0.1643 | 0.0010 | 0.0473 | -0.0197 |
| 7 | -0.2752 | 0.3817 | 0.1834 | -0.0798 | -0.1758 | -0.0739 | -0.0379 | 0.0457 | 0.5178 | 0.8221 | 0.2300 | -0.1804 |
| 8 | 0.2093 | -0.1255 | 0.1694 | -0.0800 | -0.1785 | -0.0705 | -0.1996 | -0.0475 | 0.6158 | 0.9934 | 0.0488 | -0.0247 |
| 9 | 0.2059 | -0.1535 | 0.1764 | -0.0861 | -0.1832 | -0.0678 | -0.1487 | -0.0671 | 0.6066 | 0.9712 | 0.0843 | -0.0717 |
| 10 | -0.0235 | 0.0854 | 0.2130 | -0.1392 | -0.4755 | -0.5066 | 0.1306 | 0.1613 | 0.1174 | -0.1715 | 0.0828 | -0.0561 |
| 11 | -0.2042 | 0.1736 | -0.3004 | 0.3279 | 0.0266 | 0.0186 | 0.1373 | 0.1577 | 0.6924 | 0.9728 | 0.1015 | -0.0659 |
| 12 | 0.0991 | -0.0561 | 0.1669 | -0.1554 | 0.1523 | 0.1030 | 0.1212 | 0.1207 | -0.1019 | -0.3298 | 0.0865 | -0.0698 |
| 13 | 0.1119 | -0.0291 | 0.1137 | 0.0029 | -0.6395 | -0.6491 | 0.1504 | 0.1298 | -0.0279 | -0.2067 | 0.0995 | -0.0594 |
| 14 | 0.1094 | -0.0202 | 0.0540 | -0.0902 | -0.0514 | 0.0260 | 0.1758 | 0.1638 | -0.4148 | -0.6008 | 0.1015 | -0.0590 |
| 15 | -0.1891 | 0.1484 | -0.0989 | 0.1241 | 0.4671 | 0.4327 | 0.1264 | 0.1243 | 0.1617 | 0.5101 | 0.0869 | -0.0389 |
| 16 | 0.0837 | -0.0513 | -0.1586 | 0.3675 | 0.0315 | 0.0179 | -0.0859 | -0.0667 | -0.3517 | -0.7522 | 0.0388 | -0.0387 |
| 17 | 0.1209 | -0.0204 | 0.0574 | -0.1113 | -0.4172 | -0.3549 | -0.0708 | -0.0539 | -0.2191 | -0.2628 | -0.1228 | 0.1023 |
| 18 | 0.0914 | -0.0129 | 0.0228 | 0.1562 | 0.3272 | 0.3900 | -0.0824 | -0.0419 | 0.8180 | 1.1739 | -0.1772 | 0.1504 |
| 19 | 0.1464 | 0.1244 | -0.2749 | 0.3052 | 0.3012 | 0.3888 | -0.0857 | -0.0520 | -0.0252 | -0.2647 | 0.0258 | 0.1764 |
| 20 | 0.3166 | -0.2022 | -0.1559 | 0.1891 | 0.3750 | 0.3727 | -0.0942 | -0.0459 | -0.0046 | -0.2487 | 0.1706 | -0.1218 |
| 21 | -0.1663 | 0.2872 | -0.1235 | 0.1384 | 0.2754 | 0.3022 | -0.1011 | -0.0613 | 0.4826 | 0.7161 | -0.1492 | 0.1692 |
| 22 | -0.2006 | 0.1625 | 0.0994 | -0.0465 | -0.1208 | -0.0744 | -0.0844 | -0.0661 | 0.2686 | 0.1273 | -0.2032 | 0.3552 |
| 23 | -0.2640 | 0.3071 | 0.0950 | -0.0478 | -0.4945 | -0.5091 | -0.0737 | -0.0564 | -0.7137 | -0.8441 | 0.3083 | -0.0189 |
| 24 | 0.1831 | -0.1472 | -0.1781 | 0.1439 | 0.3462 | 0.3173 | -0.0572 | -0.0446 | -0.7366 | -0.9055 | 0.2156 | -0.1343 |
| 25 | 0.2013 | -0.1322 | -0.1813 | 0.1616 | 0.1930 | 0.1514 | 0.1594 | 0.1329 | -1.2826 | -2.0489 | 0.0645 | 0.0301 |
| 26 | -0.2854 | 0.3384 | -0.1871 | 0.1770 | 0.4450 | 0.4780 | 0.1243 | 0.1226 | -0.3708 | -0.1826 | -0.1694 | 0.2069 |
| 27 | 0.2063 | -0.1329 | 0.0879 | -0.0641 | -0.1002 | -0.0586 | 0.1202 | 0.1171 | 0.7042 | 0.8925 | -0.3551 | 0.3592 |
| 28 | 0.1884 | -0.1536 | 0.0906 | -0.0558 | -0.1359 | -0.0802 | 0.1702 | 0.1565 | 0.6900 | 0.8825 | 0.1152 | -0.0453 |
| 29 | 0.1588 | -0.0675 | 0.0992 | -0.0468 | 0.0020 | -0.0290 | -0.0829 | -0.0349 | 0.2411 | 0.4319 | 0.1136 | -0.0381 |
| 30 |  |  | 0.0499 | -0.0969 | -0.1484 | -0.0783 | -0.0720 | -0.0131 | -0.1893 | 0.0428 | 0.1100 | -0.0564 |
| 31 |  |  | 0.0943 | -0.0503 | -0.1580 | -0.0807 | -0.0697 | -0.0488 | -0.2276 | -0.0388 | 0.3612 | -0.3535 |
| 32 |  |  | 0.0995 | -0.0466 | -0.1879 | -0.2039 | -0.0823 | -0.0595 | -0.4896 | -0.5912 | -0.2188 | 0.2671 |
| 33 |  |  | -0.1240 | 0.1288 | 0.2728 | 0.3185 | -0.0707 | -0.0492 | -0.4969 | -0.6035 | -0.2110 | 0.2099 |
| 34 |  |  | 0.0999 | -0.0624 | -0.1456 | -0.0871 | -0.0827 | -0.0594 | -0.4618 | -0.5620 | 0.1893 | -0.1497 |
| 35 |  |  | 0.0985 | -0.0525 | -0.4966 | -0.5127 | -0.0991 | -0.0485 | -0.5366 | -0.6389 | 0.1317 | -0.1091 |
| 36 |  |  | -0.1795 | 0.1460 | 0.3788 | 0.3164 | -0.0828 | -0.0219 | -0.1610 | 0.1026 | -0.1347 | 0.1493 |
| 37 |  |  | -0.1931 | 0.1808 | 0.2146 | 0.1714 | -0.0516 | 0.0012 | 0.1315 | 0.0617 | -0.0487 | 0.1112 |
| 38 |  |  | -0.1808 | 0.1671 | 0.4124 | 0.4635 | 0.2685 | 0.3197 | 0.1118 | 0.0193 | -0.0919 | 0.1145 |
| 39 |  |  | 0.0560 | -0.0811 | -0.1447 | -0.0679 | -0.1762 | -0.1352 | 0.1116 | 0.0211 | -0.1055 | 0.1317 |
| 40 |  |  | 0.1030 | -0.0663 | -0.1610 | -0.0798 | -0.1895 | -0.1365 | 0.4900 | 0.7635 | -0.0501 | 0.0632 |
| 41 |  |  | 0.1014 | -0.0549 | -0.1135 | -0.0432 | 0.2925 | 0.3302 | 0.1042 | 0.0225 | 0.1539 | -0.0998 |
| 42 |  |  | 0.0955 | -0.0663 | -0.1252 | -0.0624 | -0.1586 | -0.1225 | 0.1144 | 0.0266 | 0.1545 | -0.0877 |
| 43 |  |  | 0.1005 | -0.0535 | -0.0698 | -0.0336 | -0.1838 | -0.1368 |  |  | 0.1510 | -0.0926 |
| 44 |  |  | 0.0856 | -0.0753 | -0.1151 | -0.0363 | -0.3317 | -0.2617 |  |  | 0.1415 | -0.1026 |
| 45 |  |  | 0.1326 | -0.0449 | -0.1391 | -0.0181 | 0.0080 | 0.1151 |  |  | 0.4528 | -0.4180 |
| 46 |  |  | 0.1454 | -0.1197 | -0.1144 | -0.0657 |  |  |  |  | -0.1744 | 0.2405 |
| 47 |  |  | 0.1201 | -0.0425 | -0.0341 | 0.0398 |  |  |  |  | -0.2113 | 0.2203 |
| 48 |  |  | 0.1489 | -0.0298 | -0.0555 | -0.0322 |  |  |  |  | -0.0093 | -0.0127 |
| 49 |  |  | 0.1733 | -0.0717 | -0.2443 | -0.2157 |  |  |  |  | -0.2962 | 0.2971 |
| 50 |  |  |  |  | -0.0790 | -0.0705 |  |  |  |  | 0.0763 | -0.0286 |
| 51 |  |  |  |  | -0.1296 | -0.0333 |  |  |  |  | 0.0549 | -0.0585 |
| 52 |  |  |  |  | -0.0603 | -0.0190 |  |  |  |  | 0.1147 | -0.0804 |
| 53 |  |  |  |  |  |  |  |  |  |  | 0.1002 | -0.0639 |
| 54 |  |  |  |  |  |  |  |  |  |  | 0.1132 | -0.1335 |
| 55 |  |  |  |  |  |  |  |  |  |  |  |  |

**Supplementary Table 2(a):**Fukui-based local reactivity indices on each atom (with atom numbering) for complexes**1-6**by B3LYP/6-31G\*\* DFT method. Water is used as a solvent.

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|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| **No** | **7** | | **8** | | **9** | | **10** | | **11** | | **12** | |
|  |  |  |  |  |  |  |  |  |  |  |  |
| 1 | 0.0549 | 0.1792 | -0.0501 | 0.0774 | -0.0157 | 0.0304 | 0.3943 | -0.2915 | -0.1135 | 0.1995 | 0.0639 | -0.0362 |
| 2 | -0.0734 | -0.2984 | 0.0229 | -0.0436 | 0.0204 | -0.0006 | -0.1804 | 0.3128 | -0.0421 | 0.0597 | 0.0067 | 0.0612 |
| 3 | -0.1158 | -0.0164 | -0.0678 | 0.1380 | -0.1287 | 0.2141 | 0.1209 | 0.0807 | -0.0911 | 0.0988 | 0.0524 | 0.0270 |
| 4 | -0.1133 | 0.0082 | -0.1119 | 0.1361 | 0.1793 | -0.1496 | 0.0905 | 0.0372 | -0.1128 | 0.1939 | 0.1119 | 0.0212 |
| 5 | 0.0984 | 0.0227 | 0.0406 | -0.0147 | -0.1013 | 0.1885 | 0.0694 | 0.0178 | 0.1928 | -0.1066 | -0.0593 | 0.2212 |
| 6 | -0.1650 | -0.0756 | -0.1541 | 0.2228 | -0.1032 | 0.1916 | -0.1181 | 0.2305 | -0.1090 | 0.1459 | 0.0174 | 0.0446 |
| 7 | -0.1223 | 0.0263 | 0.0047 | 0.0315 | 0.0373 | -0.0262 | 0.1595 | -0.0106 | 0.1211 | -0.0607 | 0.1665 | -0.0239 |
| 8 | -0.0064 | -0.1005 | -0.1455 | 0.2357 | 0.0025 | 0.0201 | -0.2426 | 0.4084 | 0.1472 | -0.0619 | 0.1653 | -0.0167 |
| 9 | 0.1536 | 0.1012 | 0.1548 | -0.0887 | 0.1622 | -0.0913 | 0.1889 | -0.1057 | 0.1404 | -0.0554 | 0.1626 | -0.0158 |
| 10 | 0.1504 | 0.1036 | 0.1449 | -0.0818 | 0.1691 | -0.0699 | 0.2125 | -0.0986 | 0.0102 | 0.0143 | -0.0509 | 0.1895 |
| 11 | 0.1556 | 0.1131 | 0.1509 | -0.0934 | 0.1677 | -0.0773 | -0.3581 | 0.3762 | 0.0785 | -0.0774 | -0.0303 | 0.1562 |
| 12 | 0.1611 | 0.1168 | 0.1913 | -0.1547 | 0.2034 | -0.1442 | 0.1531 | -0.0445 | -0.0931 | 0.1719 | 0.2853 | 0.1310 |
| 13 | 0.2046 | -0.0117 | 0.1644 | -0.0948 | -0.0218 | 0.0647 | 0.1438 | -0.0508 | -0.0276 | 0.1086 | -0.2855 | 0.4473 |
| 14 | -0.0549 | -0.2710 | -0.0521 | 0.0527 | -0.2828 | 0.3562 | 0.1503 | -0.0469 | -0.1181 | 0.1540 | 0.1917 | -0.1050 |
| 15 | 0.0323 | 0.1459 | 0.2240 | -0.1950 | 0.2347 | -0.1904 | 0.1273 | -0.0530 | -0.0136 | 0.0787 | 0.2022 | -0.1016 |
| 16 | -0.0645 | 0.0906 | -0.3538 | 0.3662 | -0.0334 | 0.0999 | 0.0233 | 0.1035 | 0.3067 | -0.2266 |  |  |
| 17 | -0.0259 | -0.2056 | -0.2742 | 0.3669 | -0.0381 | 0.0807 | 0.0350 | 0.0709 | -0.0327 | -0.0061 |  |  |
| 18 | -0.1040 | 0.0131 | 0.1735 | -0.1527 | 0.0998 | -0.1016 | 0.0302 | 0.0638 | 0.1760 | -0.0902 |  |  |
| 19 | -0.1146 | -0.0095 | 0.1889 | -0.1423 | 0.0324 | 0.0223 |  |  | 0.1682 | -0.0671 |  |  |
| 20 | 0.0239 | -0.0315 | 0.1594 | -0.1450 | 0.1635 | -0.0871 |  |  | 0.1642 | -0.0795 |  |  |
| 21 | -0.1159 | -0.0033 | -0.1211 | 0.1590 | -0.0160 | 0.0342 |  |  | -0.0883 | 0.1870 |  |  |
| 22 | 0.1550 | 0.1111 | 0.0180 | 0.0195 | -0.1521 | 0.2219 |  |  | 0.0669 | -0.0177 |  |  |
| 23 | 0.1277 | 0.0109 | -0.0929 | 0.1362 | -0.0365 | 0.1718 |  |  | -0.1827 | 0.3088 |  |  |
| 24 | 0.1536 | 0.1026 | -0.0792 | 0.1204 | 0.1430 | -0.0490 |  |  | 0.5453 | -0.4890 |  |  |
| 25 | 0.1941 | -0.0159 | 0.0106 | 0.0158 | -0.0061 | 0.0174 |  |  | -0.1894 | 0.2910 |  |  |
| 26 | 0.1698 | 0.1104 | -0.0843 | 0.1321 | -0.0791 | 0.0474 |  |  | -0.3575 | 0.3618 |  |  |
| 27 | -0.0547 | 0.4092 | 0.1178 | -0.0656 | -0.1118 | 0.1210 |  |  | 0.2725 | -0.2050 |  |  |
| 28 | -0.2998 | 0.1829 | 0.1446 | -0.0739 | -0.1034 | 0.0828 |  |  | -0.3109 | 0.2953 |  |  |
| 29 | 0.1760 | -0.0060 | 0.1454 | -0.0849 | -0.1876 | 0.1855 |  |  | 0.2125 | -0.1818 |  |  |
| 30 | 0.1760 | -0.0066 | 0.1427 | -0.0846 | -0.1429 | 0.1388 |  |  | 0.1128 | -0.0501 |  |  |
| 31 | 0.3042 | -0.0439 | -0.0794 | 0.1182 | -0.1888 | 0.1882 |  |  | -0.3294 | 0.3328 |  |  |
| 32 | -0.1864 | 0.2750 | 0.1843 | -0.1275 | 0.0883 | -0.0758 |  |  | 0.1032 | -0.0578 |  |  |
| 33 | -0.1223 | 0.3343 | 0.0078 | 0.0170 | 0.0824 | -0.0740 |  |  | 0.1090 | -0.0638 |  |  |
| 34 | 0.1671 | -0.0520 | -0.0894 | 0.1234 | 0.0979 | -0.0696 |  |  | 0.1003 | -0.0548 |  |  |
| 35 | -0.0658 | 0.4145 | -0.1036 | 0.1474 | 0.0879 | -0.0759 |  |  | 0.0943 | -0.0410 |  |  |
| 36 | 0.3145 | -0.0217 | 0.0067 | 0.0019 | -0.3226 | 0.3406 |  |  | 0.0897 | -0.0097 |  |  |
| 37 | -0.2117 | 0.1975 | -0.1229 | 0.1509 | 0.1217 | -0.0764 |  |  |  |  |  |  |
| 38 | -0.2251 | 0.1892 | -0.0856 | 0.1193 | 0.1136 | -0.0596 |  |  |  |  |  |  |
| 39 | 0.1955 | -0.0174 | 0.1435 | -0.0823 | 0.1115 | -0.0409 |  |  |  |  |  |  |
| 40 | -0.1204 | -0.0554 | 0.1395 | -0.0810 | -0.3168 | 0.3238 |  |  |  |  |  |  |
| 41 | -0.0532 | 0.0590 | 0.1078 | -0.0773 | 0.1151 | -0.0636 |  |  |  |  |  |  |
| 42 | -0.1871 | 0.1876 | 0.1452 | -0.0943 | 0.1122 | -0.0510 |  |  |  |  |  |  |
| 43 | 0.0662 | -0.0753 | 0.2270 | -0.1812 | 0.1008 | -0.0759 |  |  |  |  |  |  |
| 44 | 0.0729 | -0.0224 | -0.2910 | 0.3419 | 0.0983 | -0.0460 |  |  |  |  |  |  |
| 45 | 0.0817 | -0.0049 | -0.3527 | 0.3679 | 0.1028 | -0.0534 |  |  |  |  |  |  |
| 46 | 0.0773 | -0.0398 | 0.1950 | -0.1421 | 0.0683 | -0.0673 |  |  |  |  |  |  |
| 47 | -0.3095 | -0.0514 | 0.1890 | -0.1479 | 0.0914 | -0.0764 |  |  |  |  |  |  |
| 48 | -0.0539 | 0.0691 | 0.1664 | -0.1493 | 0.0999 | -0.0785 |  |  |  |  |  |  |
| 49 | 0.0792 | -0.0192 |  |  | 0.0865 | -0.0742 |  |  |  |  |  |  |
| 50 | 0.0953 | -0.0058 |  |  | 0.1023 | -0.0758 |  |  |  |  |  |  |
| 51 | 0.1055 | 0.0177 |  |  | 0.0774 | -0.0567 |  |  |  |  |  |  |
| 52 | 0.0741 | -0.0460 |  |  | 0.1253 | -0.0635 |  |  |  |  |  |  |
| 53 | 0.0701 | -0.0350 |  |  | -0.1473 | 0.1489 |  |  |  |  |  |  |
| 54 | -0.0601 | 0.0356 |  |  | -0.1097 | 0.0908 |  |  |  |  |  |  |
| 55 | 0.0742 | -0.0372 |  |  | 0.0740 | -0.0841 |  |  |  |  |  |  |
| 56 | -0.2863 | 0.0014 |  |  | 0.0728 | -0.0556 |  |  |  |  |  |  |
| 57 | 0.0769 | -0.0013 |  |  |  |  |  |  |  |  |  |  |
| 58 | 0.1029 | 0.0051 |  |  |  |  |  |  |  |  |  |  |
| 59 | 0.0879 | -0.0140 |  |  |  |  |  |  |  |  |  |  |
| 60 | 0.0800 | -0.0392 |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |

**Supplementary Table 2(b)** -Fukui-based local reactivity indices on each atom (with atom numbering) for complexes **7-12** by B3LYP/6-31G\*\* DFT method. Water is used as a solvent.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **13** | | **14** | | **15** | | **16** | | **17** | | **18** | |
|  |  |  |  |  |  |  |  |  |  |  |  |
| 1 | 0.2895 | -0.0214 | -0.1583 | 0.2873 | -0.1135 | 0.1995 | -0.0948 | 0.0833 | 0.1093 | -0.0726 | 0.0347 | -0.1636 |
| 2 | -0.1318 | 0.2540 | 0.1503 | -0.4575 | -0.0421 | 0.0597 | 0.1321 | -0.1144 | -0.0761 | 0.1244 | -0.0599 | 0.0465 |
| 3 | 0.0816 | 0.0766 | -0.2989 | 0.4586 | -0.0911 | 0.0988 | 0.2206 | -0.1482 | -0.1169 | 0.1466 | 0.1359 | -0.1501 |
| 4 | 0.1772 | -0.0017 | -0.1713 | 0.7896 | -0.1128 | 0.1939 | -0.1790 | 0.2616 | -0.0522 | 0.1258 | 0.0955 | -0.1474 |
| 5 | 0.2522 | -0.1485 | -0.1548 | 0.3465 | 0.1928 | -0.1066 | -0.0346 | 0.0746 | -0.1063 | 0.1799 | 0.0880 | -0.1888 |
| 6 | -0.1902 | 0.2144 | -0.1889 | 0.4217 | -0.1090 | 0.1459 | -0.1907 | 0.3192 | 0.1712 | -0.1402 | -0.2262 | 0.0967 |
| 7 | 0.1642 | 0.0172 | 0.0768 | -0.5804 | 0.1211 | -0.0606 | -0.1429 | 0.1928 | 0.1463 | -0.0953 | -0.2598 | 0.1482 |
| 8 | 0.2390 | -0.1061 | 0.0568 | -0.5836 | 0.1472 | -0.0619 | 0.1513 | -0.0575 | 0.1525 | -0.0726 | 0.1146 | -0.1852 |
| 9 | -0.1562 | 0.4169 | 0.1718 | -0.7539 | 0.1404 | -0.0554 | 0.1493 | -0.0543 | 0.1570 | -0.0655 | 0.0972 | -0.1668 |
| 10 | 0.2385 | -0.1192 | -0.2102 | 0.6330 | 0.0102 | 0.0133 | 0.1533 | -0.0597 | 0.1623 | -0.0761 | 0.0786 | -0.1785 |
| 11 | -0.1774 | 0.2781 | 0.0573 | -0.4955 | 0.0785 | -0.0774 | 0.1856 | -0.1419 | -0.0945 | 0.1456 | -0.2287 | 0.1290 |
| 12 | -0.2285 | 0.2654 | -0.0878 | 0.3720 | -0.0931 | 0.1719 | -0.1003 | 0.1545 | 0.1212 | -0.0447 | -0.1926 | 0.1339 |
| 13 | 0.4323 | -0.1256 | 0.1127 | -0.0648 | -0.0276 | 0.1086 | 0.1241 | -0.0323 | 0.1249 | -0.0404 | -0.3333 | 0.2672 |
| 14 |  |  | -0.1229 | 0.3423 | -0.1181 | 0.1540 | -0.1121 | 0.1540 | 0.1277 | -0.0624 | 0.1362 | -0.2147 |
| 15 |  |  | 0.1307 | -0.6763 | -0.0136 | 0.0787 | -0.1913 | 0.1637 | 0.1415 | -0.0846 | 0.1374 | -0.1960 |
| 16 |  |  | -0.1315 | 0.5108 | 0.3087 | -0.2266 | 0.0937 | -0.0400 | -0.1818 | 0.2514 | -0.1939 | 0.1500 |
| 17 |  |  | -0.1948 | 0.4008 | -0.0327 | -0.0061 | 0.0822 | -0.0193 | -0.1960 | 0.2482 | -0.2200 | 0.1493 |
| 18 |  |  | 0.3209 | -1.0856 | 0.1760 | -0.0902 | 0.0833 | 0.0007 | 0.1169 | -0.0775 | -0.0493 | 0.0839 |
| 19 |  |  | -0.1738 | 0.5580 | 0.1682 | -0.0671 | -0.2492 | 0.2749 | 0.2791 | -0.0232 | 0.0235 | -0.0943 |
| 20 |  |  | -0.1798 | 0.5380 | 0.1642 | -0.0795 | -0.0108 | 0.1063 | 0.1724 | -0.0661 | 0.0354 | -0.0746 |
| 21 |  |  | 0.3659 | -0.9737 | -0.0883 | 0.1870 | -0.1412 | 0.1935 | 0.1648 | -0.0758 | 0.0357 | -0.0748 |
| 22 |  |  | -0.1172 | 0.3127 | 0.0669 | -0.0177 | 0.2251 | -0.1837 | -0.3541 | 0.3568 | -0.0591 | 0.1004 |
| 23 |  |  | -0.0988 | 0.3062 | -0.1827 | 0.3088 | -0.1208 | 0.1521 | -0.1297 | 0.1269 | 0.0348 | -0.0775 |
| 24 |  |  | -0.1007 | 0.3045 | 0.5453 | -0.4790 | 0.2499 | -0.2223 | 0.1156 | -0.0185 | 0.0260 | -0.1086 |
| 25 |  |  | -0.4026 | 1.5013 | -0.1894 | 0.2910 | 0.1541 | -0.0737 | 0.0982 | -0.0340 | 0.0403 | -0.0862 |
| 26 |  |  | 0.1161 | -0.4667 | -0.3575 | 0.3618 | 0.1662 | -0.0711 | 0.1838 | -0.1158 | -0.1129 | 0.1651 |
| 27 |  |  | 0.1156 | -0.4653 | 0.2725 | -0.2050 | 0.1665 | -0.0760 | -0.2809 | 0.3644 | -0.0773 | 0.0818 |
| 28 |  |  | 0.1175 | -0.4788 | -0.3109 | 0.2953 | -0.0898 | 0.1181 | -0.0791 | 0.0410 | -0.0799 | 0.0837 |
| 29 |  |  |  |  | 0.2125 | -0.1818 | 0.1708 | -0.0237 | -0.2528 | 0.2269 | -0.1079 | 0.1592 |
| 30 |  |  |  |  | 0.1128 | -0.0501 | 0.2939 | -0.2177 | 0.0996 | -0.0346 | 0.0616 | -0.1081 |
| 31 |  |  |  |  | -0.3294 | 0.3428 | -0.1931 | 0.2873 | 0.0496 | -0.0217 | 0.0445 | -0.1137 |
| 32 |  |  |  |  | 0.1032 | -0.0578 | -0.1440 | 0.1637 | 0.1058 | -0.0675 | 0.1299 | -0.1805 |
| 33 |  |  |  |  | 0.1090 | -0.0638 | 0.1928 | -0.1542 | 0.1209 | -0.0477 | 0.0455 | -0.1137 |
| 34 |  |  |  |  | 0.1003 | -0.0548 |  |  |  |  | 0.0144 | -0.1056 |
| 35 |  |  |  |  | 0.0943 | -0.0410 |  |  |  |  | -0.0804 | -0.0036 |
| 36 |  |  |  |  | 0.0897 | -0.0097 |  |  |  |  | -0.2793 | 0.2712 |
| 37 |  |  |  |  |  |  |  |  |  |  | 0.0671 | -0.1030 |
| 38 |  |  |  |  |  |  |  |  |  |  | 0.0374 | -0.0762 |
| 39 |  |  |  |  |  |  |  |  |  |  | 0.0364 | -0.0758 |
| 40 |  |  |  |  |  |  |  |  |  |  | 0.0114 | -0.1046 |

**Supplementary Table 2 (c)** Fukui-based local reactivity indices on each atom (with atom numbering) for complexes **13-18** by B3LYP/6-31G\*\* DFT method. Water is used as a solvent.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **19** | | **20** | | **21** | | **22** | |
|  |  |  |  |  |  |  |  |
| 1 | 0.0710 | -0.0054 | 0.1446 | -0.1124 | 0.0369 | -0.0175 | -0.1814 | 0.0949 |
| 2 | -0.0743 | 0.1004 | -0.1879 | 0.1643 | 0.1868 | -0.1517 | -0.0973 | -0.3260 |
| 3 | 0.1573 | -0.1134 | -0.1382 | 0.2449 | -0.1475 | 0.2040 | -0.1859 | -0.0409 |
| 4 | 0.1683 | -0.0452 | -0.0963 | 0.1270 | 0.0144 | 0.0110 | -0.0201 | -0.1161 |
| 5 | 0.1823 | -0.0867 | 0.2284 | -0.1875 | -0.1251 | 0.1935 | -0.2111 | 0.3810 |
| 6 | -0.1454 | 0.2243 | 0.0922 | -0.0623 | -0.0673 | 0.0989 | 0.1037 | 0.1622 |
| 7 | -0.1637 | 0.2588 | 0.0813 | 0.0120 | 0.1612 | -0.0907 | 0.1043 | -0.1026 |
| 8 | 0.1159 | -0.0825 | 0.1745 | -0.0712 | 0.1585 | -0.0808 | 0.1031 | 0.0107 |
| 9 | 0.2112 | -0.0964 | 0.1622 | -0.0753 | 0.1426 | -0.0826 | 0.0992 | -0.0073 |
| 10 | 0.1605 | -0.0773 | -0.0973 | 0.1630 | 0.1185 | -0.1432 | 0.0721 | -0.3062 |
| 11 | -0.1264 | 0.1841 | -0.3577 | 0.3679 | -0.1499 | 0.2307 | 0.1035 | -0.1371 |
| 12 | -0.1646 | 0.1663 | 0.1256 | -0.0708 | 0.1223 | -0.0801 | 0.0794 | -0.0093 |
| 13 | 0.2155 | -0.1391 | 0.1248 | -0.0644 | 0.1195 | -0.0742 | 0.0916 | -0.0097 |
| 14 | -0.3227 | 0.3641 | 0.1252 | -0.0604 | 0.1865 | -0.1345 | -0.1299 | -0.0742 |
| 15 | 0.1736 | -0.1123 | 0.2653 | -0.0285 | -0.0971 | 0.1512 | -0.1518 | 0.1797 |
| 16 | 0.1724 | -0.1371 | -0.2918 | 0.2868 | -0.0726 | 0.0962 | 0.0929 | -0.1906 |
| 17 | -0.1595 | 0.1921 | 0.1722 | -0.1221 | -0.0491 | 0.1124 | 0.0982 | 0.2346 |
| 18 | -0.1689 | 0.2352 | 0.1720 | -0.1190 | 0.1111 | -0.0698 | -0.0278 | 0.0493 |
| 19 | -0.0837 | 0.0493 | 0.2226 | -0.1463 | -0.0459 | 0.1025 | 0.1453 | 0.2488 |
| 20 | 0.0874 | -0.0238 | -0.1800 | 0.2896 | -0.1456 | 0.1821 | -0.0105 | -0.1075 |
| 21 | 0.0700 | -0.0340 | -0.1286 | 0.1802 | -0.0304 | 0.1344 | 0.1536 | -0.0458 |
| 22 | 0.0702 | -0.0338 | 0.1848 | -0.1458 | 0.1515 | -0.0812 | 0.0893 | 0.0646 |
| 23 | -0.1033 | 0.0554 | -0.1584 | 0.2317 | 0.1651 | -0.0768 | 0.1026 | -0.3085 |
| 24 | 0.0801 | -0.0288 | 0.1573 | -0.1678 | 0.1600 | -0.0672 | -0.1644 | 0.1007 |
| 25 | 0.1106 | -0.0224 | -0.1271 | 0.2371 | -0.0217 | 0.0868 | -0.1644 | -0.1502 |
| 26 | 0.0944 | -0.0341 | -0.0760 | 0.0989 | -0.2725 | 0.3600 | -0.1609 | 0.2611 |
| 27 | -0.1347 | 0.0720 | -0.0909 | 0.1450 | 0.2403 | -0.2096 | 0.1686 | -0.3544 |
| 28 | -0.1546 | 0.1391 | -0.0106 | 0.0269 | -0.0869 | 0.1275 | -0.2079 | 0.1005 |
| 29 | -0.1329 | 0.1225 | 0.1193 | -0.0753 | -0.1839 | 0.1577 | 0.0677 | 0.2330 |
| 30 | -0.1469 | 0.0984 | 0.1457 | -0.0621 | 0.0960 | -0.0314 | 0.1002 | 0.0303 |
| 31 | 0.1329 | -0.0151 | 0.1380 | -0.0611 | 0.0840 | -0.0631 | 0.0895 | -0.0020 |
| 32 | 0.1128 | -0.0505 | 0.1262 | -0.0676 | 0.0994 | -0.0455 | 0.0461 | 0.0221 |
| 33 | 0.1117 | -0.0615 | 0.4063 | -0.3733 | 0.2717 | -0.2986 | 0.2614 | 0.0744 |
| 34 | 0.1024 | -0.0246 | -0.1406 | 0.1700 | 0.2539 | -0.2953 | -0.1683 | -0.4652 |
| 35 | -0.0317 | 0.0797 | -0.1483 | 0.1694 | -0.2490 | 0.2248 | 0.0514 | 0.0555 |
| 36 | -0.0684 | 0.0593 | -0.1386 | 0.1693 | 0.0124 | -0.0493 | 0.3010 | -0.2185 |
| 37 | 0.3379 | -0.3165 |  |  | -0.2709 | 0.2540 | 0.1630 | 0.2540 |
| 38 | -0.2290 | 0.2871 |  |  | 0.1728 | -0.1300 | -0.1665 | -0.1300 |
| 39 | 0.1095 | -0.0590 |  |  | 0.1065 | -0.0685 | -0.1436 | -0.0685 |
| 40 | 0.0988 | -0.0718 |  |  | 0.0801 | -0.0304 | -0.2824 | -0.0304 |
| 41 | -0.1912 | 0.1756 |  |  | 0.0748 | -0.0879 | 0.2655 | -0.0879 |
| 42 | -0.1640 | 0.1242 |  |  | 0.1162 | -0.0704 | 0.1035 | -0.0704 |
| 43 | -0.2912 | 0.2850 |  |  | -0.3320 | 0.3383 | -0.1455 | 0.3383 |
| 44 | 0.0972 | -0.0879 |  |  | 0.1146 | -0.0776 | -0.1565 | -0.0776 |
| 45 | 0.1324 | -0.0584 |  |  | 0.0926 | -0.0820 | -0.0307 | -0.0820 |
| 46 | 0.1121 | -0.0782 |  |  | 0.1086 | -0.0790 | 0.2650 | -0.0790 |
| 47 | 0.0813 | -0.0895 |  |  | -0.3735 | 0.3697 | 0.1638 | 0.3697 |
| 48 | 0.1067 | -0.0698 |  |  | 0.1262 | -0.0742 | 0.1695 | -0.0742 |
| 49 | 0.0850 | -0.0415 |  |  | 0.0720 | -0.0906 | 0.1480 | -0.0906 |
| 50 | 0.1045 | -0.0692 |  |  | 0.0890 | -0.0813 |  |  |
| 51 | 0.1012 | -0.0620 |  |  | -0.3499 | 0.4145 |  |  |
| 52 | 0.0889 | -0.0423 |  |  | 0.0967 | -0.0676 |  |  |
| 53 |  |  |  |  | -0.3650 | 0.3617 |  |  |
| 54 |  |  |  |  | 0.1057 | -0.0696 |  |  |
| 55 |  |  |  |  | 0.0723 | -0.0904 |  |  |
| 56 |  |  |  |  | 0.1183 | -0.0758 |  |  |
| 57 |  |  |  |  | -0.3344 | 0.3394 |  |  |
| 58 |  |  |  |  | 0.1059 | -0.0758 |  |  |
| 59 |  |  |  |  | 0.1111 | -0.0778 |  |  |
| 60 |  |  |  |  | 0.1040 | -0.0798 |  |  |

**Supplementary Table 2 (d):** Fukui-based local reactivity indices on each atom (with atom numbering) for complexes **19-22** by B3LYP/6-31G\*\* DFT method. Water is used as a solvent.

.

The optimized output Cartesian coordinates of all complexes (1-22) with B3LYP/6-31G\*\* method is given here.

**Supplementary Table 3:**

**Complex 1**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -2.11251 0.45466 -0.01859 | 0.0296 |
| C -1.60959 -0.88545 -0.06511 | 0.1728 |
| C 0.57487 -0.16786 -0.04428 | 0.1002 |
| C 0.10006 1.17758 -0.14671 | 0.0815 |
| N -0.34321 -1.14748 -0.05049 | -0.0828 |
| N -1.21861 1.44094 -0.10051 | -0.1152 |
| N 0.91821 2.23889 -0.30613 | -0.2852 |
| H 0.51836 3.15925 -0.2186 | 0.2093 |
| H 1.91111 2.06676 -0.18165 | 0.2059 |
| N -3.43327 0.79404 0.05533 | -0.0235 |
| C -3.81861 2.1746 -0.22673 | -0.2044 |
| H -3.23274 2.56615 -1.05505 | 0.0991 |
| H -4.87553 2.18312 -0.49873 | 0.1119 |
| H -3.67384 2.82905 0.64159 | 0.1094 |
| C -4.40039 0.05267 0.87048 | -0.1891 |
| H -3.91545 -0.73744 1.43524 | 0.0837 |
| H -4.85469 0.74386 1.58662 | 0.1209 |
| H -5.19334 -0.38379 0.25736 | 0.0914 |
| Cl -2.69255 -2.29169 -0.31211 | 0.1464 |
| C 2.00275 -0.61173 0.02106 | 0.3166 |
| O 2.2555 -1.82873 0.06872 | -0.1663 |
| N 2.9188 0.40661 0.03418 | -0.2006 |
| N 5.06081 1.20665 0.17202 | -0.2640 |
| H 4.66807 2.12203 0.02907 | 0.1831 |
| H 6.05662 1.10127 0.06408 | 0.2013 |
| N 4.76478 -1.08379 0.1145 | -0.2854 |
| H 5.75696 -1.23172 0.20531 | 0.2063 |
| H 4.1001 -1.85221 0.1196 | 0.1884 |
| C 4.22862 0.14407 0.09971 | 0.1588 |

**Complex 2**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -0.70564 -3.0099 -0.03609 | -0.0224 |
| C -0.29261 -1.66578 -0.13999 | 0.0370 |
| C 1.01911 -1.26074 0.20982 | 0.0499 |
| C 1.83803 -2.31289 0.70871 | 0.1658 |
| C 1.42056 -3.63677 0.82032 | -0.1241 |
| C 0.13577 -4.01441 0.44377 | -0.1035 |
| C -2.41056 -1.80895 -0.84514 | 0.1834 |
| H 2.12691 -4.36245 1.20285 | 0.1694 |
| H -0.1941 -5.04223 0.52218 | 0.1764 |
| H -2.58497 -3.88301 -0.5906 | 0.2130 |
| C 1.57557 0.03773 0.09243 | -0.3004 |
| C 2.91131 0.25025 0.51325 | 0.1669 |
| C 3.63593 -0.79179 0.9978 | 0.1137 |
| N -1.39084 -0.93552 -0.63457 | 0.0540 |
| N -2.01262 -3.06463 -0.46964 | -0.0989 |
| C -1.6538 0.43507 -0.73618 | -0.1586 |
| C -3.02064 0.76415 -0.61287 | 0.0574 |
| C -3.98061 -0.19992 -0.79305 | 0.0228 |
| N -3.59203 -1.44536 -1.45909 | -0.2749 |
| O 3.13499 -2.06035 1.10488 | -0.1559 |
| C -3.41314 2.17392 -0.22734 | -0.1235 |
| H -3.27041 2.82314 -1.09825 | 0.0994 |
| H -4.4966 2.18924 -0.00127 | 0.0950 |
| N -2.62215 2.73685 0.86818 | -0.1781 |
| C -2.83933 4.16851 1.00568 | -0.1813 |
| C -2.86078 2.04181 2.12595 | -0.1871 |
| H -2.59558 4.67478 0.06802 | 0.0879 |
| H -2.18541 4.56768 1.78579 | 0.0906 |
| H -3.88226 4.4278 1.2738 | 0.0992 |
| H -2.6772 0.97414 1.99821 | 0.0499 |
| H -2.17865 2.41974 2.89215 | 0.0943 |
| H -3.89717 2.17071 2.49338 | 0.0995 |
| C 3.51751 1.63457 0.45684 | -0.1240 |
| H 2.99194 2.26989 1.17784 | 0.0999 |
| H 4.5741 1.58936 0.78442 | 0.0985 |
| N 3.37615 2.2589 -0.85607 | -0.1795 |
| C 4.17689 1.59526 -1.87683 | -0.1931 |
| C 3.65142 3.68783 -0.80568 | -0.1808 |
| H 3.91096 0.53857 -1.93315 | 0.0560 |
| H 3.97549 2.04757 -2.85058 | 0.1030 |
| H 5.26378 1.66789 -1.68127 | 0.1014 |
| H 3.46233 4.13203 -1.78585 | 0.0955 |
| H 4.69603 3.9198 -0.52312 | 0.1005 |
| H 2.9879 4.16924 -0.08328 | 0.0856 |
| H 4.65819 -0.74092 1.34282 | 0.1326 |
| H 1.03531 0.85283 -0.35906 | 0.1454 |
| H -0.87087 1.11495 -0.46276 | 0.1201 |
| H -5.01492 -0.10555 -0.49223 | 0.1489 |
| H -3.45431 -1.31194 -2.46924 | 0.1733 |

**Complex 3**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -3.4362 0.04811 0.1746 | -0.1376 |
| C -2.04442 0.07918 -0.07271 | 0.0340 |
| C -1.28254 -1.08619 -0.26319 | -0.0433 |
| C -2.00465 -2.28964 -0.22528 | -0.1704 |
| C -3.38914 -2.33229 0.01184 | 0.1152 |
| C -4.11229 -1.17115 0.22106 | 0.0923 |
| C -2.89704 2.10684 0.23057 | -0.1758 |
| H -3.86451 -3.30518 0.02815 | -0.1785 |
| H -5.17818 -1.1939 0.41226 | -0.1832 |
| C 0.23209 -1.09719 -0.43464 | -0.4755 |
| C 0.77665 -2.49131 -0.41989 | 0.0261 |
| C -0.11877 -3.4925 -1.05296 | 0.1523 |
| N -1.71164 1.44096 -0.03788 | -0.6395 |
| N -3.93375 1.329 0.36827 | -0.0514 |
| C -0.4626 2.12315 -0.37055 | 0.4671 |
| C 0.40444 2.47175 0.84915 | 0.0315 |
| N -2.94484 3.49576 0.24107 | -0.4172 |
| H -3.88132 3.80447 0.46787 | 0.3272 |
| O -1.40334 -3.51797 -0.38912 | 0.3012 |
| C 1.55689 3.41766 0.49131 | 0.3750 |
| H 1.12824 4.34729 0.10167 | 0.2754 |
| H 2.10797 3.68897 1.41214 | -0.1208 |
| N 2.45557 2.88826 -0.53463 | -0.4945 |
| C 3.231 3.94921 -1.16611 | 0.3462 |
| C 3.33266 1.8407 -0.02299 | 0.1930 |
| H 2.56039 4.69192 -1.60461 | 0.4450 |
| H 3.84036 3.53005 -1.97046 | -0.1002 |
| H 3.90834 4.46886 -0.46227 | -0.1359 |
| H 2.76127 0.99536 0.36267 | 0.0020 |
| H 3.9587 1.46436 -0.83538 | -0.1484 |
| H 3.99938 2.20396 0.78244 | -0.1580 |
| C 1.83297 -2.88863 0.56344 | -0.1879 |
| H 1.40784 -2.85532 1.58005 | 0.2728 |
| H 2.1288 -3.94121 0.39032 | -0.1456 |
| N 2.99631 -1.99582 0.55925 | -0.4966 |
| C 3.77015 -2.12348 -0.67048 | 0.3788 |
| C 3.83567 -2.19977 1.73345 | 0.2146 |
| H 3.12852 -1.93831 -1.5342 | 0.4124 |
| H 4.57662 -1.3864 -0.6785 | -0.1447 |
| H 4.22047 -3.12701 -0.78719 | -0.1610 |
| H 4.27555 -3.21347 1.77981 | -0.1135 |
| H 4.65602 -1.47783 1.72927 | -0.1252 |
| H 3.24966 -2.04202 2.64194 | -0.0698 |
| H 0.26267 -4.5113 -0.98094 | -0.1151 |
| H 0.50151 -0.60832 -1.38456 | -0.1391 |
| H -0.73464 3.04112 -0.8997 | -0.1144 |
| H -2.26111 3.94205 0.83919 | -0.0341 |
| H 0.10351 1.5174 -1.07263 | -0.0555 |
| H -0.21091 2.96205 1.61255 | -0.2443 |
| H 0.7778 1.55519 1.31444 | -0.0790 |
| H -0.29274 -3.25341 -2.11303 | -0.1296 |
| H 0.71579 -0.50943 0.34945 | -0.0603 |

**Complex 4**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -1.14944 -0.67791 -0.11663 | 0.0751 |
| C -2.33805 0.09216 -0.11756 | -0.0548 |
| C -1.14963 2.08498 -0.20224 | -0.2238 |
| C 0.10939 1.43461 -0.01682 | -0.0723 |
| C 0.11083 0.0059 -0.0469 | 0.0896 |
| C 1.33953 -0.66609 -0.02165 | 0.0567 |
| C 2.52088 0.07998 0.043 | -0.0379 |
| C 1.37374 2.07763 0.15299 | -0.1996 |
| H 1.36096 -1.74505 -0.04963 | -0.1487 |
| N -2.30408 1.44364 -0.2259 | 0.1306 |
| N 2.52461 1.43436 0.16976 | 0.1373 |
| C -5.4123 -1.68216 0.78847 | 0.1212 |
| C -3.94037 -1.79809 0.37193 | 0.1504 |
| C -4.78433 0.42832 -0.1675 | 0.1758 |
| C -5.9455 -0.56918 -0.12317 | 0.1264 |
| H -5.94469 -2.62841 0.6788 | -0.0859 |
| H -5.48334 -1.37496 1.83649 | -0.0708 |
| H -3.81692 -2.5067 -0.45205 | -0.0824 |
| H -3.29595 -2.12817 1.18824 | -0.0857 |
| H -4.83009 1.13923 0.66506 | -0.0942 |
| H -4.74441 1.01168 -1.0882 | -0.1011 |
| H -6.86671 -0.11312 0.24397 | -0.0844 |
| H -6.1416 -0.96487 -1.12452 | -0.0737 |
| N -3.59143 -0.42943 -0.04622 | -0.0572 |
| C 3.9547 -1.94807 -0.14444 | 0.1594 |
| C 5.46903 -2.07157 -0.36275 | 0.1243 |
| C 6.03706 -0.87287 0.41265 | 0.1202 |
| C 5.00477 0.2338 0.16203 | 0.1702 |
| H 3.37719 -2.33861 -0.98754 | -0.0829 |
| H 3.63307 -2.49066 0.75529 | -0.0720 |
| H 5.70013 -1.97343 -1.42776 | -0.0697 |
| H 5.85978 -3.0323 -0.02325 | -0.0823 |
| H 6.08232 -1.10521 1.48116 | -0.0707 |
| H 7.03985 -0.58775 0.08925 | -0.0827 |
| H 4.93242 0.95336 0.9784 | -0.0991 |
| H 5.23141 0.7992 -0.75075 | -0.0828 |
| N 3.74747 -0.50824 0.01327 | -0.0516 |
| N -1.23714 3.45579 -0.34338 | 0.2685 |
| H -0.45672 3.91513 -0.79257 | -0.1762 |
| H -2.1526 3.75587 -0.64743 | -0.1895 |
| N 1.46542 3.46291 0.2838 | 0.2925 |
| H 0.75086 3.89026 0.85868 | -0.1586 |
| H 2.40384 3.73888 0.54182 | -0.1838 |
| C -1.12723 -2.08515 -0.27256 | -0.3317 |
| N -1.04447 -3.23221 -0.4237 | 0.0080 |

**Complex 5**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -4.59189 -0.55916 -0.16115 | 0.0358 |
| C -3.84665 0.61357 0.11932 | 0.2794 |
| C -4.48131 1.83824 0.33456 | -0.2197 |
| C -5.87246 1.86591 0.2729 | -0.6798 |
| C -5.97064 -0.53868 -0.23312 | -0.4322 |
| C -2.35312 -1.07551 -0.31326 | 0.1643 |
| H -3.9164 2.73845 0.54145 | 0.5177 |
| H -6.42014 2.78356 0.43346 | 0.6158 |
| H -6.57073 -1.40941 -0.4518 | 0.6066 |
| H -3.89588 -2.47454 -0.72917 | 0.1174 |
| H -1.76 0.91383 0.15138 | 0.6924 |
| C 4.24266 -0.10407 0.09713 | -0.1019 |
| C 4.86724 -1.37441 0.054 | -0.0279 |
| C 6.24979 -1.52941 -0.05228 | -0.4148 |
| C 7.01078 -0.37247 -0.1136 | 0.1617 |
| C 6.38731 0.88469 -0.06927 | -0.3517 |
| C 5.01333 1.05376 0.03481 | -0.2191 |
| C 2.65187 -1.53736 0.22064 | 0.8180 |
| H 6.7204 -2.50445 -0.08547 | -0.0252 |
| H 8.08728 -0.4122 -0.19548 | -0.0046 |
| H 4.5753 2.04069 0.06561 | 0.4826 |
| H 3.89444 -3.27537 0.12738 | 0.2686 |
| N -3.66775 -1.57828 -0.33218 | -0.7137 |
| N -2.52299 0.26083 0.08421 | -0.7366 |
| N 2.86757 -0.24869 0.20011 | -1.2826 |
| N 3.82324 -2.27028 0.13331 | -0.3708 |
| N 7.23939 2.08921 -0.13649 | 0.7042 |
| N -8.04379 0.77801 -0.06961 | 0.6900 |
| C -6.59271 0.70557 -0.00462 | 0.2411 |
| O -8.65568 -0.26129 -0.32633 | -0.1893 |
| O -8.58681 1.86501 0.13453 | -0.2276 |
| O 6.68657 3.18054 -0.09272 | -0.4896 |
| O 8.44965 1.92614 -0.23207 | -0.4969 |
| C 0.16215 -1.30788 -0.12134 | -0.4618 |
| C -1.21377 -1.90845 0.19503 | -0.5366 |
| C 1.31421 -2.19809 0.35932 | -0.1610 |
| H -1.29473 -2.90245 -0.25971 | 0.1315 |
| H 0.2744 -0.3298 0.35417 | 0.1118 |
| H 0.25255 -1.14053 -1.19837 | 0.1116 |
| H 1.16217 -2.45888 1.41511 | 0.4900 |
| H -1.30613 -2.05936 1.28629 | 0.1042 |
| H 1.31712 -3.14579 -0.19194 | 0.1144 |

**Complex 6**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom X Y Z | | | | Mulliken charges |
| C | 0.79922 | -0.81159 | -1.41536 | -0.046489 |
| C | 0.59595 | -0.54042 | 1.08406 | -0.049281 |
| C | -0.2137 | -1.95213 | -1.47537 | -0.117515 |
| C | -0.09801 | -1.87098 | 1.39806 | -0.296852 |
| C | -1.44098 | -2.10698 | 0.69209 | -0.026295 |
| H | 0.32255 | 0.13716 | -1.65673 | 0.158614 |
| H | 2.15526 | -1.42669 | 0.06443 | 0.228328 |
| H | -0.10479 | 0.27656 | 0.91055 | 0.157807 |
| H | 0.60084 | -2.68866 | 1.19674 | 0.131896 |
| H | 0.2303 | -2.90148 | -1.15439 | 0.11939 |
| H | 1.59197 | -0.98056 | -2.14564 | 0.129095 |
| H | 1.24365 | -0.25024 | 1.9097 | 0.137216 |
| H | -0.50949 | -2.0792 | -2.51549 | 0.16352 |
| H | -0.29019 | -1.9117 | 2.47426 | 0.129198 |
| H | -1.69698 | -3.17415 | 0.76238 | 0.116156 |
| H | -2.21149 | -1.55881 | 1.22855 | 0.146143 |
| N | -1.43655 | -1.67313 | -0.71458 | -0.434375 |
| N | 1.50088 | -0.61782 | -0.10981 | -0.330288 |
| C | 2.41188 | 0.60151 | -0.20678 | -0.287315 |
| C | 5.93097 | 0.45939 | 0.25632 | 0.001407 |
| C | 3.59606 | 0.17523 | 0.29223 | 0.130513 |
| C | 3.99752 | -1.12051 | 0.89425 | -0.582488 |
| S | 5.78773 | -1.19009 | 0.7159 | 0.193111 |
| H | 4.6168 | 1.95821 | -0.24222 | 0.226507 |
| H | 3.77615 | -1.21573 | 1.95962 | 0.144579 |
| N | 4.75024 | 1.02679 | 0.13504 | -0.312867 |
| C | 7.20846 | 1.14399 | -0.10742 | -0.270393 |
| H | 7.32168 | 2.06179 | 0.47669 | 0.144161 |
| H | 7.22338 | 1.41391 | -1.16798 | 0.146739 |
| H | 8.06293 | 0.49972 | 0.09738 | 0.141034 |
| C | -2.61607 | -1.67289 | -1.46184 | 0.489765 |
| O | -2.66591 | -1.99626 | -2.63441 | -0.377725 |
| N | -3.79256 | -1.33289 | -0.79212 | -0.456808 |
| H | -4.58085 | -1.47082 | -1.40984 | 0.241594 |
| C | -4.01048 | -0.40605 | 0.26293 | 0.069868 |
| C | -4.92602 | -0.78212 | 1.25229 | -0.061931 |
| C | -5.2034 | 0.04705 | 2.33251 | -0.066631 |
| C | -4.53484 | 1.26198 | 2.46288 | -0.096061 |
| C | -3.62428 | 1.64825 | 1.4874 | -0.025208 |
| C | -3.37208 | 0.84718 | 0.36481 | -0.078096 |
| H | -5.40026 | -1.75309 | 1.16651 | 0.101039 |
| H | -5.9228 | -0.26642 | 3.0805 | 0.102602 |
| H | -4.72635 | 1.90724 | 3.31201 | 0.101105 |
| H | -3.11284 | 2.59842 | 1.56402 | 0.114117 |
| C | -2.5484 | 1.41649 | -0.75054 | 0.400392 |
| O | -2.7302 | 1.18954 | -1.92173 | -0.338876 |
| O | -1.61394 | 2.27218 | -0.28884 | -0.34543 |
| C | -0.87481 | 3.03097 | -1.28904 | -0.025901 |
| C | 0.2777 | 3.72207 | -0.59296 | -0.314542 |
| H | -1.5732 | 3.73448 | -1.75091 | 0.117371 |
| H | -0.52945 | 2.34499 | -2.06325 | 0.12998 |
| H | 0.78527 | 4.37563 | -1.30892 | 0.095013 |
| H | -0.07855 | 4.33832 | 0.23669 | 0.097193 |
| H | 1.00088 | 2.98546 | -0.23211 | 0.135914 |
|  |  |  |  |  |

**Complex 7**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -7.08222 0.66887 0.18996 | 0.0549 |
| C -7.40989 -0.71558 0.17877 | -0.0734 |
| C -8.73877 -1.14875 0.24948 | -0.1158 |
| C -9.72953 -0.18789 0.33594 | -0.1133 |
| C -9.43377 1.20414 0.34881 | 0.0984 |
| C -8.11068 1.62767 0.27422 | -0.1650 |
| C -5.65924 0.75463 0.09928 | -0.1223 |
| C -5.17565 -0.54105 0.03726 | -0.0064 |
| H -8.98882 -2.20327 0.23702 | 0.1536 |
| H -10.76738 -0.49811 0.39814 | 0.1504 |
| H -7.87489 2.68689 0.27979 | 0.1556 |
| H -5.07823 1.66444 0.08898 | 0.1611 |
| H -6.11393 -2.42069 0.05955 | 0.2046 |
| C 1.34371 -0.74542 -0.4656 | -0.0549 |
| C 0.78063 0.5592 -0.5046 | 0.0323 |
| C -0.61017 0.71002 -0.39687 | -0.0645 |
| C -1.41067 -0.42186 -0.26662 | -0.0259 |
| C -0.82961 -1.71618 -0.24092 | -0.1040 |
| C 0.54222 -1.88275 -0.34009 | -0.1146 |
| C 3.02755 0.73115 -0.70027 | 0.0239 |
| C 1.86746 1.47252 -0.66563 | -0.1159 |
| H -1.05703 1.69855 -0.41963 | 0.1550 |
| H -1.47658 -2.5729 -0.14199 | 0.1277 |
| H 0.97439 -2.87619 -0.31615 | 0.1536 |
| H 3.35168 -1.37888 -0.68791 | 0.1941 |
| H 1.81894 2.54726 -0.7353 | 0.1698 |
| N -6.23406 -1.41964 0.08676 | -0.0547 |
| N -10.48616 2.12017 0.50725 | -0.2998 |
| H -11.36697 1.80509 0.12267 | 0.1760 |
| H -10.27327 3.0522 0.17715 | 0.1760 |
| C -3.81996 -1.12278 -0.06068 | 0.3042 |
| O -3.67044 -2.34584 -0.05048 | -0.1864 |
| N -2.80553 -0.21347 -0.16062 | -0.1223 |
| H -3.08527 0.75621 -0.18049 | 0.1671 |
| N 2.70949 -0.61243 -0.56519 | -0.0658 |
| C 4.39666 1.27557 -0.89503 | 0.3145 |
| O 4.54459 2.33959 -1.50088 | -0.2117 |
| N 5.46123 0.58055 -0.41565 | -0.2251 |
| H 6.36322 0.99972 -0.619 | 0.1955 |
| C 5.53081 -0.46152 0.60764 | -0.1204 |
| C 6.70766 -0.16972 1.54682 | -0.0532 |
| N 7.9634 0.01041 0.81485 | -0.1871 |
| H 4.61177 -0.4795 1.19322 | 0.0662 |
| H 5.65188 -1.44871 0.14686 | 0.0729 |
| H 6.76452 -0.9769 2.29608 | 0.0817 |
| H 6.49154 0.75792 2.08195 | 0.0773 |
| C 8.66474 -1.27619 -1.23445 | -0.3095 |
| C 8.51141 -1.25994 0.28817 | -0.0539 |
| H 9.48153 -1.46216 0.75867 | 0.0792 |
| H 9.34216 -0.48894 -1.57291 | 0.0953 |
| H 9.06719 -2.23831 -1.56669 | 0.1055 |
| H 7.70026 -1.12348 -1.72554 | 0.0741 |
| H 7.85821 -2.0855 0.59014 | 0.0701 |
| C 8.94619 0.79325 1.57799 | -0.0601 |
| H 8.41723 1.64129 2.02047 | 0.0742 |
| C 10.09359 1.32485 0.72144 | -0.2863 |
| H 9.35771 0.20268 2.41607 | 0.0769 |
| H 10.76062 1.93761 1.33396 | 0.1029 |
| H 10.69156 0.51883 0.2896 | 0.0879 |
| H 9.71139 1.94229 -0.0957 | 0.0800 |

**Complex 8**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C 4.28807 0.16629 -0.07989 | -0.0501 |
| C 4.49099 -1.01937 0.67702 | 0.0229 |
| C 5.79272 -1.32239 1.10991 | -0.0678 |
| C 6.83302 -0.4781 0.76578 | -0.1119 |
| C 6.62003 0.69148 -0.00101 | 0.0406 |
| C 5.33106 1.02347 -0.42228 | -0.1541 |
| C 2.28706 -0.86765 0.1579 | 0.0047 |
| C 3.2154 -1.64969 0.81267 | -0.1455 |
| H 5.98121 -2.20747 1.70739 | 0.1548 |
| H 7.83703 -0.69777 1.1101 | 0.1449 |
| H 5.16486 1.91044 -1.02241 | 0.1509 |
| H 2.52828 0.87922 -1.02466 | 0.1913 |
| H 2.99674 -2.54919 1.36629 | 0.1644 |
| N 2.93994 0.24386 -0.36133 | -0.0521 |
| C 7.78336 1.55296 -0.37124 | 0.2240 |
| N 7.49669 2.90936 -0.48094 | -0.3538 |
| N 8.9692 1.14697 -0.63489 | -0.2742 |
| H 9.00177 0.12964 -0.64125 | 0.1735 |
| H 8.32587 3.46992 -0.62519 | 0.1889 |
| H 6.86187 3.28499 0.20858 | 0.1594 |
| C -1.39242 -0.13637 -0.33405 | -0.1211 |
| C -1.95193 -1.4228 -0.31129 | 0.0180 |
| C -1.08635 -2.5179 -0.14239 | -0.0929 |
| C 0.27877 -2.33531 -0.0052 | -0.0792 |
| C 0.84611 -1.05052 -0.00688 | 0.0106 |
| C -0.02417 0.03739 -0.17381 | -0.0843 |
| H -2.0239 0.72749 -0.49048 | 0.1178 |
| H -1.49816 -3.52203 -0.12438 | 0.1446 |
| H 0.92199 -3.20156 0.09491 | 0.1454 |
| H 0.36766 1.04876 -0.16176 | 0.1427 |
| N -3.31285 -1.67046 -0.49967 | -0.0794 |
| H -3.53549 -2.58587 -0.85804 | 0.1843 |
| C -6.71209 0.76348 0.09745 | 0.0078 |
| C -6.721 -0.29964 -0.81319 | -0.0894 |
| C -5.58943 -1.07791 -1.01517 | -0.1036 |
| C -4.40818 -0.82703 -0.30022 | 0.0067 |
| C -4.39882 0.23397 0.6218 | -0.1229 |
| C -5.5288 1.01528 0.80256 | -0.0856 |
| H -7.6045 -0.49775 -1.40883 | 0.1435 |
| H -5.60891 -1.87773 -1.7485 | 0.1395 |
| H -3.5155 0.42657 1.21571 | 0.1078 |
| H -5.52117 1.83666 1.50772 | 0.1452 |
| C -7.89772 1.63665 0.3272 | 0.2270 |
| N -7.72537 2.80236 0.82777 | -0.2910 |
| N -9.11622 1.10015 -0.08776 | -0.3527 |
| H -8.61423 3.28514 0.96767 | 0.1950 |
| H -9.93572 1.61602 0.19887 | 0.1890 |
| H -9.2235 0.10115 0.012 | 0.1664 |

**Complex 9**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -5.01458 0.29224 0.3422 | -0.0157 |
| C -4.04502 -0.69617 0.01408 | 0.0204 |
| C -4.45494 -2.03618 -0.0449 | -0.1287 |
| C -5.78477 -2.35753 0.20407 | 0.1793 |
| C -6.72527 -1.36496 0.51827 | -0.1013 |
| C -6.34301 -0.0282 0.5914 | -0.1032 |
| C -3.04274 1.37139 0.09244 | 0.0373 |
| C -2.77887 0.00044 -0.15605 | 0.0025 |
| H -3.7737 -2.84612 -0.26228 | 0.1622 |
| H -7.75786 -1.64199 0.70917 | 0.1691 |
| H -7.06974 0.73793 0.83831 | 0.1677 |
| H -4.80823 2.36887 0.72436 | 0.2034 |
| N -4.39314 1.53117 0.35575 | -0.0218 |
| O -6.13033 -3.68763 0.13317 | -0.2828 |
| H -7.06642 -3.77686 0.33527 | 0.2347 |
| C -2.06298 2.37635 0.04393 | -0.0334 |
| C -0.75409 1.96561 -0.21537 | -0.0381 |
| C -0.44435 0.57418 -0.48317 | 0.0998 |
| C -1.47204 -0.40731 -0.49224 | 0.0324 |
| H 0.19368 3.94524 -0.05136 | 0.1635 |
| C 0.35597 2.89446 -0.24243 | -0.0160 |
| C 0.90234 0.22506 -0.73435 | -0.1521 |
| C 1.62341 2.48126 -0.50015 | -0.0365 |
| H 2.46159 3.16631 -0.52309 | 0.1430 |
| N 1.92008 1.17316 -0.75212 | -0.0061 |
| C 3.30323 0.73907 -0.92144 | -0.0791 |
| C 3.93198 0.2292 0.38765 | -0.1118 |
| C 6.13919 -0.0588 1.38025 | -0.1034 |
| C 7.60705 -0.36035 1.07011 | -0.1876 |
| C 7.76664 -1.76453 0.47561 | -0.1429 |
| C 6.82411 -1.94695 -0.71976 | -0.1888 |
| H 7.97286 0.3858 0.35619 | 0.0883 |
| H 6.03733 0.9696 1.73755 | 0.0824 |
| H 8.80468 -1.94122 0.17827 | 0.0979 |
| H 7.14476 -1.30165 -1.54493 | 0.0879 |
| C -2.43633 3.81936 0.28428 | -0.3226 |
| H -3.48746 4.00013 0.04331 | 0.1217 |
| H -1.85712 4.49825 -0.34506 | 0.1136 |
| H -2.27937 4.12519 1.326 | 0.1115 |
| C -1.14097 -1.83197 -0.84852 | -0.3168 |
| H -0.47457 -1.87532 -1.71668 | 0.1151 |
| H -0.63413 -2.35859 -0.02862 | 0.1122 |
| H -2.03119 -2.4005 -1.10576 | 0.1008 |
| H 3.32278 -0.03749 -1.69026 | 0.0983 |
| H 3.89249 1.57787 -1.29568 | 0.1028 |
| H 3.2946 -0.56108 0.82017 | 0.0683 |
| H 3.9346 1.05556 1.10376 | 0.0914 |
| H 6.8531 -2.97917 -1.08274 | 0.0999 |
| H 7.52681 -2.51185 1.2428 | 0.0865 |
| H 8.20094 -0.25687 1.98375 | 0.1023 |
| H 5.79304 -0.7226 2.19747 | 0.0774 |
| H 1.21603 -0.78688 -0.92972 | 0.1253 |
| N 5.3074 -0.21395 0.18269 | -0.1473 |
| C 5.38684 -1.58129 -0.34154 | -0.1097 |
| H 4.74247 -1.66316 -1.22027 | 0.0740 |
| H 5.00548 -2.30723 0.40435 | 0.0728 |

**Complex 10**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -2.31665 -0.20225 0.00063 | 0.3943 |
| N -1.72829 -1.41071 -0.02471 | -0.1804 |
| C -0.39804 -1.41046 -0.02867 | 0.1209 |
| C 0.36771 -0.24948 -0.0067 | 0.0905 |
| C -0.34861 0.97342 -0.00294 | 0.0694 |
| N -1.68947 0.9747 0.00248 | -0.1181 |
| H 0.09436 -2.37914 -0.0533 | 0.1595 |
| N 0.26823 2.18009 0.01617 | -0.2426 |
| H 1.24899 2.26478 -0.19518 | 0.1889 |
| H -0.31953 2.99075 -0.09554 | 0.2125 |
| C -3.81766 -0.1848 0.02733 | -0.3581 |
| H -4.175 -0.6503 0.95031 | 0.1531 |
| H -4.19059 0.83588 -0.03278 | 0.1438 |
| H -4.21201 -0.77798 -0.80102 | 0.1503 |
| C 1.81131 -0.28714 0.01609 | 0.1273 |
| N 2.95357 -0.2409 0.87255 | 0.0233 |
| N 2.9245 -1.07422 -0.36781 | 0.0350 |
| N 2.95225 0.41107 -0.47111 | 0.0302 |

**Complex 11**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -0.68096 -1.06314 -0.01966 | -0.1135 |
| C -2.06994 -0.97554 -0.01736 | -0.0421 |
| C -2.71467 0.26091 0.00186 | -0.0911 |
| C -1.91893 1.41283 0.01845 | -0.1128 |
| C -0.5342 1.33567 0.01659 | 0.1928 |
| C 0.11198 0.08901 -0.00181 | -0.1090 |
| H -0.21992 -2.0443 -0.03846 | 0.1211 |
| H -2.65744 -1.8864 -0.03167 | 0.1472 |
| H -2.39361 2.38967 0.03348 | 0.1404 |
| H 0.06526 2.2367 0.02936 | 0.0102 |
| C -4.23537 0.39648 0.00365 | 0.0785 |
| N -5.04538 -0.81464 -0.00002 | -0.0931 |
| H -4.85901 -1.37966 -0.82173 | -0.0276 |
| H -4.85212 -1.38889 0.81371 | -0.1181 |
| H -4.52823 0.99612 -0.86565 | -0.0136 |
| H -4.52642 0.99017 0.87754 | 0.3067 |
| C 2.38735 -1.09647 0.02397 | -0.0327 |
| C 1.58221 0.01954 -0.00186 | 0.1760 |
| N 3.57616 1.06462 -0.02633 | 0.1682 |
| H 2.08604 -2.13106 0.05121 | 0.1642 |
| N 2.31938 1.188 -0.02841 | -0.0883 |
| S 4.02309 -0.63275 0.01203 | 0.0669 |

**Complex 12**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -0.39116 -0.79901 -0.0077 | 0.0639 |
| C -0.06848 0.57922 -0.00948 | 0.0067 |
| C -2.27208 1.06421 0.00956 | 0.0524 |
| C -2.57682 -0.3059 -0.00068 | 0.1119 |
| C 2.05356 -0.34181 0.00682 | -0.0593 |
| C 1.35348 0.82867 -0.00971 | 0.0174 |
| H -3.06718 1.80301 0.02255 | 0.1665 |
| H -3.60896 -0.64122 -0.00149 | 0.1653 |
| H 3.12626 -0.4617 0.00183 | 0.1626 |
| N -1.63618 -1.25331 -0.00457 | -0.0509 |
| N -1.02014 1.51912 0.00677 | -0.0303 |
| S 1.04897 -1.79317 0.00633 | 0.2853 |
| N 1.83889 2.1249 -0.0832 | -0.2855 |
| H 1.15181 2.8183 0.18125 | 0.1917 |
| H 2.74553 2.28508 0.32879 | 0.2022 |

**Complex 13**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C 1.28328 1.64527 0.00007 | 0.2991 |
| N 0.00094 1.86295 -0.00015 | -0.1318 |
| C -0.71756 0.71482 -0.00023 | 0.0817 |
| C -0.25441 -0.59831 -0.00037 | 0.1772 |
| C 1.16494 -0.85392 -0.00002 | 0.2522 |
| N 1.85382 0.40893 0.00017 | -0.1902 |
| H 1.96792 2.48707 0.00031 | 0.1642 |
| H 2.86296 0.32788 0.00004 | 0.2390 |
| O 1.78881 -1.89037 0.00008 | -0.1562 |
| H -2.75525 1.37743 0.00048 | 0.2385 |
| N -1.33703 -1.4749 -0.0001 | -0.1774 |
| N -2.09895 0.61287 0.00008 | -0.2285 |
| C -2.36253 -0.73091 0.00031 | 0.4323 |

**Complex 14**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Atom X Y Z | | | | Mulliken charges |
| C | 2.98842 | 2.57652 | -0.01486 | 0.0986 |
| C | 3.67689 | 1.35765 | -0.00793 | -0.15568 |
| C | 2.87927 | 0.2284 | -0.00154 | -0.052579 |
| C | 0.99982 | 1.48636 | -0.00965 | 0.491877 |
| H | 3.53173 | 3.51595 | -0.01978 | 0.129408 |
| H | 4.75499 | 1.3095 | -0.0075 | 0.121822 |
| N | 1.66484 | 2.65854 | -0.01583 | -0.328344 |
| N | 1.54767 | 0.26985 | -0.00226 | -0.379794 |
| N | -0.36583 | 1.58869 | -0.012 | -0.4192 |
| H | -0.73513 | 2.53064 | -0.016 | 0.248597 |
| C | -2.66846 | -1.44633 | -0.0052 | -0.360704 |
| C | -1.32051 | 0.5879 | -0.00546 | 0.186726 |
| C | -3.39135 | -0.25074 | -0.00729 | 0.155287 |
| H | -3.0302 | -2.46079 | 0.01459 | 0.126549 |
| N | -2.57777 | 0.88961 | -0.00065 | -0.391133 |
| S | -0.94781 | -1.13917 | -0.01474 | 0.270483 |
| C | -4.79164 | -0.07977 | -0.01279 | 0.023627 |
| N | -5.32191 | 1.19167 | 0.14668 | -0.426867 |
| H | -4.66055 | 1.94074 | -0.01248 | 0.213786 |
| H | -6.22144 | 1.35351 | -0.28681 | 0.19952 |
| C | -5.75529 | -1.22266 | -0.03508 | -0.239117 |
| H | -6.6236 | -0.98662 | -0.66034 | 0.10018 |
| H | -5.29646 | -2.12825 | -0.43306 | 0.114643 |
| H | -6.13756 | -1.45336 | 0.96844 | 0.125851 |
| C | 3.46345 | -1.17127 | 0.01058 | 0.754334 |
| F | 3.04992 | -1.88293 | -1.057 | -0.198664 |
| F | 3.08213 | -1.84878 | 1.11229 | -0.199206 |
| F | 4.80912 | -1.15491 | -0.00945 | -0.21 |

**Complex 15**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C 2.03304 -1.79972 -0.47052 | -0.0948 |
| C 1.65069 -0.48117 -0.23014 | 0.1321 |
| C 2.63106 0.52464 0.08722 | 0.2206 |
| C 3.99457 0.11756 0.09734 | -0.1790 |
| C 4.33003 -1.19046 -0.15567 | -0.0346 |
| C 3.3765 -2.16663 -0.4305 | -0.1907 |
| H 1.27143 -2.53607 -0.67652 | -0.1429 |
| H 4.7835 0.82373 0.31665 | 0.1513 |
| H 3.68699 -3.18626 -0.61778 | 0.1493 |
| C -1.97882 0.09047 -0.12651 | 0.1533 |
| C -1.5 1.36914 -0.40492 | 0.1856 |
| C -2.36314 2.44406 -0.57294 | -0.1003 |
| C -3.73419 2.21142 -0.47318 | 0.1241 |
| C -4.22156 0.9334 -0.19863 | -0.1121 |
| C -3.35292 -0.1416 0.00554 | -0.1913 |
| C -0.83011 -0.86866 -0.10827 | 0.0937 |
| C -0.00004 1.33393 -0.52407 | 0.0822 |
| H -1.98799 3.4378 -0.79135 | 0.0833 |
| H -4.43193 3.02899 -0.61216 | -0.2492 |
| H -5.28834 0.75932 -0.12964 | -0.0108 |
| F 5.63652 -1.54669 -0.13217 | -0.1412 |
| N 0.3066 -0.07752 -0.27773 | 0.2251 |
| O -0.85338 -2.0767 -0.0055 | -0.1208 |
| C -3.96461 -1.46554 0.35078 | 0.2499 |
| O -4.92275 -1.92991 -0.21532 | 0.1541 |
| O -3.37296 -2.0421 1.41023 | 0.1662 |
| H -3.78562 -2.91105 1.52634 | 0.1665 |
| C 0.79121 2.21731 0.44143 | -0.0898 |
| C 2.24869 1.84453 0.42771 | 0.1708 |
| H 0.66449 3.26919 0.16311 | 0.2939 |
| C 3.25009 2.86791 0.87636 | -0.1931 |
| H 3.99665 3.07833 0.10022 | -0.1440 |
| H 2.76242 3.8123 1.12519 | 0.1928 |
| H 3.80484 2.53797 1.76331 | -0.0948 |
| H 0.37393 2.11264 1.4551 | 0.1321 |
| H 0.3044 1.58201 -1.55035 | 0.2206 |

**Complex 16**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C 3.49575 0.60375 -0.10282 | 0.1093 |
| C 2.4698 -0.38026 -0.17622 | -0.0761 |
| C 2.85084 -1.7254 -0.25704 | -0.1169 |
| C 4.17983 -2.09626 -0.23975 | -0.0522 |
| C 5.16844 -1.10688 -0.14442 | -0.1064 |
| C 4.84049 0.25456 -0.07684 | 0.1712 |
| C 1.24224 0.29999 -0.12559 | 0.1463 |
| H 4.43732 -3.14595 -0.30144 | 0.1525 |
| H 6.20978 -1.40342 -0.12998 | 0.1570 |
| H 5.61763 1.00551 -0.01485 | 0.1623 |
| H 0.91337 2.24744 0.46567 | -0.0945 |
| F 1.86704 -2.66355 -0.34193 | 0.1212 |
| N 2.8971 1.85444 -0.10881 | 0.1249 |
| N 1.48896 1.67033 -0.14873 | 0.1277 |
| C 3.38172 3.0086 0.61884 | 0.1415 |
| H 4.45293 3.10463 0.44663 | -0.1818 |
| H 2.8961 3.907 0.23353 | -0.1960 |
| H 3.1976 2.92926 1.70003 | 0.1169 |
| C -4.88297 -0.06245 -0.22909 | 0.2791 |
| C -5.00214 -1.42728 0.00879 | 0.1724 |
| C -3.86866 -2.1831 0.29326 | 0.1648 |
| C -2.64768 -1.54218 0.3429 | -0.3541 |
| C -2.46026 -0.16726 0.12987 | -0.1297 |
| C -3.63777 0.55497 -0.16797 | 0.1156 |
| H -5.75239 0.53402 -0.47088 | 0.0982 |
| H -5.97487 -1.90119 -0.03503 | 0.1838 |
| H -3.91288 -3.24747 0.48384 | -0.2809 |
| F -1.55833 -2.30855 0.62712 | -0.0791 |
| Cl -3.59035 2.26311 -0.55428 | -0.2528 |
| C -1.13522 0.50045 0.31419 | 0.0996 |
| O -1.02006 1.63011 0.79125 | 0.0496 |
| N -0.0307 -0.20853 -0.12227 | 0.1058 |
| H -0.12044 -1.19555 -0.32144 | 0.1209 |

**Complex 17**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C 2.65116 -0.04803 0.4177 | 0.0347 |
| C 2.71214 1.24332 0.95139 | -0.0590 |
| C 3.69185 2.15264 0.5575 | 0.1359 |
| C 4.64341 1.78274 -0.38966 | 0.0955 |
| C 4.60981 0.50428 -0.94218 | 0.0880 |
| C 3.62039 -0.37304 -0.53038 | -0.2262 |
| H 1.97598 1.53332 1.69392 | -0.2599 |
| H 3.71348 3.14531 0.99183 | 0.1146 |
| H 5.41077 2.4823 -0.69981 | 0.0972 |
| H 5.33259 0.17824 -1.67988 | 0.0786 |
| F 3.59507 -1.61634 -1.07874 | -0.2297 |
| H -4.66757 1.68091 -2.36421 | -0.1926 |
| H -5.96164 1.13043 -1.29744 | -0.3333 |
| H -5.18926 2.69398 -1.01376 | 0.1362 |
| C -3.99199 1.03577 -0.417 | 0.1374 |
| C -3.33574 1.59103 0.64268 | -0.1939 |
| C -2.42456 0.69832 1.28548 | -0.2200 |
| C -2.38317 -0.54591 0.72579 | -0.0493 |
| S -3.48834 -0.62716 -0.632 | 0.0235 |
| H -3.49663 2.6154 0.95578 | 0.0354 |
| H -1.82174 0.9709 2.14347 | 0.0357 |
| C -5.00621 1.66308 -1.32377 | -0.0591 |
| C -1.53834 -1.73377 1.1211 | 0.0348 |
| H -2.17733 -2.59731 1.33068 | 0.0260 |
| H -1.04661 -1.48412 2.06616 | 0.0403 |
| H -0.97414 -2.55622 -0.66201 | -0.1129 |
| N -0.52158 -2.17695 0.1612 | -0.0773 |
| C 0.47258 -1.17764 -0.23611 | -0.0799 |
| C 1.58953 -1.04347 0.81799 | -0.1079 |
| H 0.9232 -1.5161 -1.17167 | 0.0616 |
| H 0.03118 -0.18747 -0.42665 | 0.0445 |
| H 1.1615 -0.73284 1.77515 | 0.1299 |
| H 2.02996 -2.03232 0.96757 | 0.0455 |

**Complex 18**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -0.12889 2.01359 -0.10781 | 0.0347 |
| C 0.96861 1.09167 -0.10761 | -0.0590 |
| C 0.60258 -0.27626 -0.01488 | 0.1359 |
| C -1.60937 0.27545 0.12362 | 0.0955 |
| H 2.65386 2.4814 -0.21538 | 0.0880 |
| C 2.33415 1.44628 -0.17812 | -0.2262 |
| C 1.62867 -1.25504 -0.04585 | -0.2599 |
| C 2.95552 -0.89124 -0.14609 | 0.1146 |
| C 3.31998 0.49151 -0.20105 | 0.0972 |
| H 1.32071 -2.28938 0.00916 | 0.0786 |
| N -0.687 -0.6795 0.10595 | -0.2297 |
| N -1.37971 1.61353 0.00675 | -0.1926 |
| N 0.08445 3.36484 -0.19324 | -0.3333 |
| H -0.74587 3.91239 -0.36074 | 0.1362 |
| H 0.92393 3.69162 -0.64202 | 0.1374 |
| O 3.99544 -1.76459 -0.20315 | -0.1939 |
| O 4.63061 0.87397 -0.34579 | -0.2200 |
| C 3.70563 -3.15779 -0.19608 | -0.0493 |
| H 4.66818 -3.6604 -0.27277 | 0.0235 |
| H 3.20892 -3.4576 0.73264 | 0.0354 |
| H 3.07876 -3.43552 -1.04944 | 0.0357 |
| C 5.47146 0.66662 0.79434 | -0.0591 |
| H 5.55913 -0.39469 1.03616 | 0.0348 |
| H 6.45066 1.06065 0.52272 | 0.0260 |
| H 5.08802 1.21426 1.66304 | 0.0403 |
| C -4.00006 0.86549 0.45246 | -0.1129 |
| C -5.23853 0.45076 -0.34095 | -0.0773 |
| C -4.54576 -1.8594 -0.28572 | -0.0799 |
| C -3.29279 -1.48904 0.50587 | -0.1079 |
| H -3.64909 1.84685 0.146 | 0.0616 |
| H -6.06325 1.12751 -0.09952 | 0.0445 |
| H -6.47089 -1.18044 -0.45187 | 0.1299 |
| H -4.86536 -2.86626 -0.00226 | 0.0455 |
| H -3.49515 -1.61842 1.57916 | 0.0144 |
| N -2.92549 -0.10048 0.23966 | -0.0805 |
| N -5.61832 -0.91358 0.02763 | -0.2795 |
| H -2.45244 -2.12247 0.23451 | 0.0651 |
| H -4.29018 -1.87148 -1.36065 | 0.0385 |
| H -5.01487 0.55422 -1.41825 | 0.0365 |
| H -4.2584 0.90353 1.521 | 0.0114 |

**Complex 19**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C -1.73706 2.19816 0.02603 | 0.0730 |
| C -2.65211 1.14335 0.11213 | -0.0743 |
| C -2.13942 -0.1912 0.00385 | 0.1573 |
| C 0.03261 0.56765 -0.22821 | 0.1683 |
| H -4.49226 2.28504 0.41551 | 0.1823 |
| C -4.05081 1.30333 0.29237 | -0.1458 |
| C -3.00922 -1.27541 0.06837 | -0.1637 |
| C -4.38548 -1.09702 0.24664 | 0.1159 |
| C -4.90212 0.2152 0.35733 | 0.2112 |
| H -2.5727 -2.2618 -0.00429 | 0.1606 |
| N -0.77131 -0.43683 -0.13525 | -0.1264 |
| N -0.36672 1.89273 -0.119 | -0.1646 |
| H 0.15684 2.58165 -0.64547 | 0.2155 |
| N -2.0095 3.57569 -0.01639 | -0.3227 |
| H -1.83859 4.06098 0.86272 | 0.1736 |
| H -2.95411 3.77045 -0.32218 | 0.1724 |
| O -5.29214 -2.11813 0.34709 | -0.1596 |
| O -6.23411 0.44465 0.60668 | -0.1689 |
| C -4.80573 -3.45082 0.31119 | -0.0832 |
| H -5.67966 -4.09008 0.42863 | 0.0876 |
| H -4.31699 -3.67733 -0.64332 | 0.0700 |
| H -4.10376 -3.64363 1.13 | 0.0702 |
| C -7.13761 0.09539 -0.44581 | -0.1033 |
| H -7.12779 -0.97885 -0.64003 | 0.0801 |
| H -8.12823 0.39686 -0.10491 | 0.1107 |
| H -6.89053 0.6395 -1.3652 | 0.0945 |
| C 2.38218 1.1933 0.22042 | -0.1349 |
| C 3.6987 1.20712 -0.56071 | -0.1548 |
| C 3.15241 -0.99937 -1.46638 | -0.1329 |
| C 1.84446 -1.00122 -0.68096 | -0.1469 |
| H 2.56376 0.78515 1.22745 | 0.1329 |
| H 4.44258 1.75631 0.01129 | 0.1128 |
| H 3.56623 -2.00303 -1.53578 | 0.1117 |
| H 1.98584 -1.50469 0.28621 | 0.1024 |
| N 1.38625 0.37682 -0.47959 | -0.0317 |
| N 4.15507 -0.15288 -0.81667 | -0.0684 |
| C 5.4408 -0.62878 -0.66583 | 0.3379 |
| O 5.73881 -1.7684 -0.99312 | -0.2290 |
| H 7.44597 -0.10375 -0.3664 | 0.1085 |
| H 6.40182 1.31123 -0.39449 | 0.0988 |
| C 6.48373 0.28462 -0.02811 | -0.1912 |
| C 6.44356 0.27029 1.51556 | -0.1640 |
| C 6.73807 -1.10276 2.12667 | -0.2912 |
| H 5.46736 0.62467 1.86576 | 0.0972 |
| H 7.17933 0.99592 1.87846 | 0.1324 |
| H 6.7045 -1.05536 3.21842 | 0.1121 |
| H 6.0186 -1.85461 1.79578 | 0.0813 |
| H 7.73134 -1.45511 1.83467 | 0.1067 |
| H 2.96699 -0.62758 -2.48304 | 0.0850 |
| H 1.07237 -1.54407 -1.22165 | 0.1045 |
| H 2.02069 2.21355 0.34054 | 0.1012 |
| H 3.54175 1.73385 -1.51304 | 0.0889 |

**Complex 20**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C 3.88368 -0.69035 -0.01224 | 0.1446 |
| C 3.63208 0.69995 0.03008 | -0.1879 |
| C 4.752 1.54066 0.05497 | -0.1382 |
| C 6.00826 0.96005 0.03225 | -0.0963 |
| C 6.14202 -0.44402 -0.01422 | 0.2284 |
| C 1.45278 -0.14091 0.01413 | 0.0922 |
| C 2.22525 0.9926 0.04474 | 0.0813 |
| H 4.64048 2.61947 0.09423 | 0.1745 |
| H 6.8976 1.57811 0.05106 | 0.1622 |
| N 5.08246 -1.25856 -0.03355 | -0.0973 |
| C 7.49514 -1.10253 -0.05392 | -0.3577 |
| H 8.30135 -0.38499 0.10641 | 0.1256 |
| H 7.55548 -1.88273 0.708 | 0.1248 |
| H 7.65009 -1.58678 -1.02272 | 0.1252 |
| S 2.39677 -1.62194 -0.02617 | 0.2653 |
| N 1.66491 2.31456 0.08769 | -0.2918 |
| H 2.04084 2.89511 -0.65687 | 0.1722 |
| H 1.87823 2.77408 0.96937 | 0.1720 |
| C -0.02813 -0.33237 0.00301 | 0.2226 |
| O -0.49938 -1.45948 0.00337 | -0.1800 |
| N -0.75589 0.82895 -0.01391 | -0.1286 |
| H -0.1919 1.68011 -0.01544 | 0.1848 |
| C -3.04858 -0.09489 -0.02598 | -0.1584 |
| C -4.41793 0.16247 -0.04801 | 0.1573 |
| C -4.91715 1.46284 -0.07756 | -0.1271 |
| C -4.01879 2.52617 -0.08581 | -0.0760 |
| C -2.65154 2.29137 -0.0629 | -0.0909 |
| C -2.15005 0.98016 -0.03291 | -0.0106 |
| H -2.67321 -1.10582 -0.01215 | 0.1193 |
| H -5.98444 1.63714 -0.1027 | 0.1457 |
| H -4.38653 3.5452 -0.11332 | 0.1380 |
| H -1.95839 3.12621 -0.0721 | 0.1262 |
| C -5.37649 -0.99669 0.02181 | 0.4063 |
| F -5.65399 -1.33625 1.30362 | -0.1406 |
| F -4.89129 -2.10322 -0.57677 | -0.1484 |
| F -6.56121 -0.71054 -0.56553 | -0.1388 |

**Complex 21**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C 2.55743 -0.4974 0.00709 | 0.0369 |
| C 3.1579 0.50399 -0.8081 | 0.1868 |
| C 4.54106 0.70979 -0.75225 | -0.1475 |
| C 5.36716 -0.03401 0.0873 | 0.0144 |
| C 4.77563 -1.02823 0.89054 | -0.1251 |
| C 3.41237 -1.24393 0.83944 | -0.0673 |
| H 4.94756 1.46478 -1.41415 | 0.1612 |
| H 5.38535 -1.61433 1.5666 | 0.1585 |
| H 2.99819 -2.01898 1.47223 | 0.1426 |
| C 6.81272 0.20642 0.13668 | 0.1185 |
| C 7.50019 1.35913 -0.21505 | -0.1499 |
| H 7.74562 -1.70079 0.89568 | 0.1223 |
| H 7.15376 2.31538 -0.5722 | 0.1195 |
| H 9.59107 1.73098 -0.14177 | 0.1865 |
| C 7.84223 -0.68065 0.55599 | -0.0971 |
| N 8.81328 1.10767 0.00066 | -0.0726 |
| N 9.04736 -0.13443 0.4693 | -0.0491 |
| C -1.5948 -1.04173 -0.25423 | 0.1111 |
| C 1.1062 -0.74364 -0.01816 | -0.0459 |
| C 0.44928 -1.68756 0.81162 | -0.1456 |
| C -0.90383 -1.83323 0.69638 | -0.0304 |
| H 0.99661 -2.26458 1.54397 | 0.1515 |
| H -1.44868 -2.51465 1.33818 | 0.1651 |
| N 0.37422 -0.01236 -0.86999 | 0.1600 |
| N -0.94097 -0.15889 -1.00416 | -0.0217 |
| O 2.46265 1.27643 -1.65474 | -0.2725 |
| H 1.5089 0.99732 -1.59008 | 0.2403 |
| N -2.98835 -1.16219 -0.39139 | -0.0869 |
| C -3.39345 -2.51732 -0.80186 | -0.1839 |
| H -3.33235 -2.64358 -1.89322 | 0.0960 |
| H -2.7336 -3.25421 -0.34671 | 0.0840 |
| H -4.40775 -2.73905 -0.47873 | 0.0994 |
| C -4.30398 1.62462 0.79756 | 0.2717 |
| C -6.08822 -0.02565 -0.04323 | 0.2539 |
| C -5.19973 -0.27913 -1.28364 | -0.2390 |
| C -3.68297 -0.05769 -1.11602 | 0.0124 |
| C -3.48084 1.32988 -0.47288 | -0.2709 |
| H -6.2857 1.48269 1.33928 | 0.1728 |
| H -5.50609 0.44503 -2.04459 | 0.1065 |
| H -3.25336 -0.00737 -2.12605 | 0.0802 |
| H -2.42603 1.51752 -0.2811 | 0.0748 |
| H -3.78665 2.05252 -1.23645 | 0.1162 |
| C -4.2836 3.14548 1.04311 | -0.3320 |
| H -4.85584 3.39761 1.94251 | 0.1146 |
| H -3.26181 3.50768 1.18716 | 0.0926 |
| H -4.73219 3.67173 0.19853 | 0.1086 |
| C -3.69558 0.94083 2.04736 | -0.3735 |
| H -4.332 1.11645 2.92092 | 0.1262 |
| H -3.57581 -0.13216 1.91473 | 0.0720 |
| H -2.7086 1.36013 2.26727 | 0.0890 |
| N -5.71174 1.27797 0.52719 | -0.3499 |
| H -5.42504 -1.26308 -1.6998 | 0.0967 |
| C -6.04979 -1.19664 0.97021 | -0.3650 |
| H -6.47971 -2.10454 0.53345 | 0.1057 |
| H -5.04089 -1.4254 1.30737 | 0.0723 |
| H -6.65126 -0.94377 1.8491 | 0.1183 |
| C -7.54591 0.12136 -0.52253 | -0.3344 |
| H -7.89213 -0.78762 -1.0236 | 0.1059 |
| H -8.21214 0.30622 0.32661 | 0.1111 |
| H -7.63383 0.96413 -1.21052 | 0.1040 |

**Complex 22**

|  |  |
| --- | --- |
| Atom X Y Z | Mulliken charges |
| C 1.00187 -4.05194 -1.60875 | -0.1814 |
| C -0.23491 -4.22909 -0.7008 | -0.0973 |
| C 0.09581 -2.1818 0.53832 | -0.1859 |
| C 1.58039 -2.29112 0.10523 | -0.0201 |
| C 1.66862 -2.68303 -1.38384 | -0.2113 |
| H 0.70863 -4.13905 -2.65864 | 0.1039 |
| H -1.00026 -4.81495 -1.21533 | 0.1043 |
| H 2.07625 -3.07346 0.68555 | 0.1031 |
| H 2.71462 -2.71323 -1.70194 | 0.0992 |
| H 1.16814 -1.91441 -1.9759 | 0.0721 |
| H 1.71501 -4.85826 -1.40933 | 0.1035 |
| H 0.03375 -4.79605 0.21142 | 0.0794 |
| H -0.00141 -2.55853 1.57488 | 0.0916 |
| N -0.79331 -2.92096 -0.36589 | -0.1289 |
| C -2.16129 -2.98653 0.14066 | -0.1518 |
| H -2.20652 -3.43814 1.15138 | 0.0929 |
| H -2.71877 -3.658 -0.5221 | 0.0982 |
| C -2.8942 -0.79539 -0.93651 | -0.0278 |
| C -2.84346 -1.64004 0.18049 | 0.1453 |
| C -3.48019 -1.14544 1.31313 | -0.0105 |
| C -4.1091 0.73726 0.21859 | 0.1536 |
| H -2.39704 -1.08633 -1.85831 | 0.0893 |
| H -3.47841 -1.71993 2.23813 | 0.1026 |
| N -3.50892 0.37884 -0.93979 | -0.1646 |
| N -4.11334 0.02752 1.35832 | -0.1644 |
| N -4.77013 1.92538 0.20397 | -0.1607 |
| H -4.6537 2.46592 -0.63683 | 0.1686 |
| C -5.35559 2.53309 1.38225 | -0.2079 |
| H -4.59709 2.87225 2.09783 | 0.0677 |
| H -5.95547 3.38932 1.07083 | 0.1002 |
| H -5.99954 1.81766 1.89569 | 0.0895 |
| H -0.20738 -1.13485 0.53659 | 0.0461 |
| C 4.25839 -0.04652 1.14821 | 0.2614 |
| C 3.80814 1.21442 0.76527 | -0.1683 |
| C 2.55319 1.25611 0.15986 | 0.0514 |
| C 2.35917 -1.02166 0.37128 | 0.3010 |
| H 4.41427 2.09129 0.94004 | 0.1630 |
| N 1.83292 0.1304 -0.03177 | -0.1665 |
| N 3.55714 -1.16097 0.961 | -0.1436 |
| O 5.45963 -0.16377 1.74073 | -0.2824 |
| H 5.57893 -1.10702 1.92363 | 0.2655 |
| C 1.94364 2.50005 -0.29938 | 0.1035 |
| C 2.42682 3.78774 -0.24593 | -0.1455 |
| C 1.5356 4.74206 -0.79817 | -0.1565 |
| C 0.38339 4.16859 -1.26563 | -0.0307 |
| S 0.36316 2.45741 -1.04224 | 0.2650 |
| H 3.38965 4.04527 0.17496 | 0.1668 |
| H 1.73944 5.80342 -0.8465 | 0.1695 |
| H -0.45873 4.65664 -1.73253 | 0.1480 |