# Use of Benzothiophene Functions to Improve the Photovoltaic Efficacy of Cyanopyridinone-based Organic Chromophores: A DFT Study

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**Table S1:** Cartesian coordinates of **A1R**.

| Atoms | X-axis | Y-axis | Z-axis |
|---|---|---|---|
| C | 3.554564 | 0.173873 | 0.636222 |
| C | 2.685239 | -0.75321 | 0.059318 |
| C | 3.1078 | -2.098 | -0.06336 |
| C | 4.381502 | -2.4919 | 0.298815 |
| C | 5.274451 | -1.54354 | 0.823552 |
| C | 4.833622 | -0.21908 | 0.997317 |
| H | 3.240655 | 1.195518 | 0.829167 |
| H | 4.695095 | -3.52633 | 0.173479 |
| C | 0.864566 | -2.02684 | -0.67197 |
| C | -0.30399 | -2.51871 | -1.25537 |
| C | -0.3707 | -3.84982 | -1.63564 |
| C | 0.723553 | -4.71846 | -1.47292 |
| C | 1.921165 | -4.20966 | -0.94428 |
| C | 1.985636 | -2.88221 | -0.56575 |
| H | -1.15559 | -1.8699 | -1.43825 |
| H | 2.786655 | -4.85917 | -0.82903 |
| C | 1.263863 | -0.66609 | -0.29555 |
| C | 1.017283 | 4.574545 | -1.19346 |

| | | | |
|---|---|---|---|
| C | -0.19006 | 4.030082 | -0.72707 |
| C | -0.25833 | 2.682741 | -0.42953 |
| C | 0.86855 | 1.838774 | -0.5575 |
| C | 2.04841 | 2.368282 | -1.08399 |
| C | 2.119216 | 3.720173 | -1.38248 |
| H | -1.06479 | 4.665421 | -0.5969 |
| H | 2.906663 | 1.733063 | -1.28468 |
| C | -1.39109 | 1.868581 | -0.00548 |
| C | -2.67179 | 2.241243 | 0.353218 |
| C | -3.57326 | 1.263877 | 0.806599 |
| C | -3.12989 | -0.06597 | 0.921229 |
| C | -1.84131 | -0.43626 | 0.569285 |
| C | -0.96541 | 0.521032 | 0.05531 |
| H | -2.96776 | 3.287948 | 0.327477 |
| H | -3.81435 | -0.82937 | 1.285134 |
| H | -1.53174 | -1.46842 | 0.705017 |
| C | 0.464568 | 0.4573 | -0.27143 |
| H | 5.497348 | 0.5093 | 1.458264 |
| C | 0.637717 | -6.11701 | -1.86722 |
| C | 1.687629 | -6.96218 | -2.19199 |
| S | -0.89495 | -6.92265 | -1.96633 |
| C | 1.254479 | -8.24095 | -2.53069 |
| H | 2.72619 | -6.64832 | -2.21318 |
| C | -0.13021 | -8.41875 | -2.47177 |
| H | 1.917378 | -9.04784 | -2.83084 |
| C | 6.620711 | -1.94459 | 1.205427 |
| C | 7.056236 | -3.22298 | 1.51929 |
| S | 7.904101 | -0.78221 | 1.304543 |
| C | 8.407282 | -3.25709 | 1.851119 |
| H | 6.406588 | -4.09183 | 1.539502 |
| C | 9.049446 | -2.01701 | 1.797923 |
| H | 8.938884 | -4.15833 | 2.144007 |
| C | 1.133178 | 5.99174 | -1.50546 |
| C | 2.295964 | 6.745065 | -1.55823 |
| S | -0.27013 | 6.942777 | -1.87093 |
| C | 2.050691 | 8.078289 | -1.87398 |
| H | 3.280482 | 6.34333 | -1.34159 |
| C | 0.703264 | 8.387945 | -2.07842 |
| H | 2.824384 | 8.837491 | -1.94946 |
| C | -4.92979 | 1.642897 | 1.174173 |
| C | -5.61412 | 2.780868 | 0.775024 |
| S | -5.88785 | 0.64849 | 2.224163 |
| C | -6.89815 | 2.843359 | 1.307623 |
| H | -5.20365 | 3.521403 | 0.096367 |
| C | -7.23971 | 1.763241 | 2.125531 |
| H | -7.60036 | 3.648362 | 1.109097 |
| H | -1.282 | -4.2187 | -2.10151 |
| H | 3.037435 | 4.120167 | -1.80513 |

| | | | |
|---|---|---|---|
| C | 0.32879 | 9.717764 | -2.39217 |
| C | -0.83805 | 10.40634 | -2.65287 |
| H | 1.222985 | 10.33965 | -2.42477 |
| C | -8.52338 | 1.718144 | 2.723679 |
| C | -9.22939 | 0.862997 | 3.544149 |
| H | -9.07883 | 2.610661 | 2.436651 |
| C | -0.68755 | -9.67961 | -2.80016 |
| C | -1.94347 | -10.2451 | -2.86928 |
| H | 0.117301 | -10.3642 | -3.06628 |
| C | 10.42317 | -1.92642 | 2.132336 |
| C | 11.38171 | -0.9382 | 2.216799 |
| H | 10.79039 | -2.91826 | 2.394942 |
| C | -8.64486 | -0.3951 | 4.020814 |
| C | -10.5763 | 1.209 | 3.936339 |
| C | -3.14737 | -9.4749 | -2.53985 |
| C | -2.07713 | -11.6254 | -3.27447 |
| C | 12.71957 | -1.28307 | 2.63888 |
| C | 11.07131 | 0.457349 | 1.889078 |
| C | -0.77918 | 11.82536 | -2.91724 |
| C | -2.13896 | 9.729043 | -2.6675 |
| C | -1.94419 | 12.50063 | -3.16732 |
| C | -3.26221 | 11.86188 | -3.18433 |
| C | 0.527256 | 12.55106 | -2.91439 |
| H | 1.02105 | 12.4644 | -1.93996 |
| H | 1.208132 | 12.13761 | -3.66685 |
| H | 0.396308 | 13.6129 | -3.12973 |
| C | -11.2749 | 0.343933 | 4.735607 |
| C | -10.7308 | -0.92595 | 5.222735 |
| C | -11.2026 | 2.486928 | 3.480135 |
| H | -10.6114 | 3.351249 | 3.802471 |
| H | -11.269 | 2.522296 | 2.386865 |
| H | -12.2114 | 2.604445 | 3.879664 |
| C | -3.32921 | -12.1756 | -3.3418 |
| C | -4.55515 | -11.4396 | -3.02364 |
| C | -0.87346 | -12.4424 | -3.61693 |
| H | -0.32119 | -11.9949 | -4.45077 |
| H | -0.18821 | -12.5069 | -2.76432 |
| H | -1.14679 | -13.4593 | -3.90395 |
| C | 13.65859 | -0.29099 | 2.735164 |
| C | 13.385 | 1.115181 | 2.42948 |
| C | 13.07798 | -2.69524 | 2.97223 |
| H | 12.47342 | -3.06526 | 3.808008 |
| H | 12.90063 | -3.3578 | 2.117921 |
| H | 14.12843 | -2.78557 | 3.254229 |
| N | -3.26921 | 10.49072 | -2.93067 |
| N | -9.42604 | -1.21436 | 4.824518 |
| N | -4.37706 | -10.1108 | -2.64035 |
| N | 12.08329 | 1.398856 | 2.01731 |

| | | | |
|---|---|---|---|
| O | -4.28983 | 12.48094 | -3.40492 |
| O | -5.66196 | -11.9482 | -3.08707 |
| O | 14.23402 | 1.985752 | 2.524794 |
| O | -11.3698 | -1.68583 | 5.931316 |
| O | -7.50675 | -0.75124 | 3.739541 |
| O | -2.26998 | 8.528413 | -2.46008 |
| O | -3.11233 | -8.30361 | -2.1821 |
| O | 9.965228 | 0.822968 | 1.509079 |
| C | -8.81528 | -2.46013 | 5.27607 |
| H | -7.91934 | -2.24454 | 5.863086 |
| H | -9.54737 | -2.98753 | 5.884378 |
| H | -8.52922 | -3.06864 | 4.414879 |
| C | -5.55234 | -9.31321 | -2.30689 |
| H | -5.49231 | -8.97548 | -1.26941 |
| H | -5.60073 | -8.43517 | -2.95514 |
| H | -6.43109 | -9.93913 | -2.44964 |
| C | 11.73752 | 2.777272 | 1.686988 |
| H | 10.89969 | 3.107116 | 2.30547 |
| H | 12.61387 | 3.394749 | 1.874577 |
| H | 11.44304 | 2.847643 | 0.636935 |
| C | -4.54471 | 9.78247 | -2.93462 |
| H | -4.71015 | 9.31069 | -1.96308 |
| H | -5.32912 | 10.50806 | -3.14056 |
| H | -4.53594 | 9.004542 | -3.70184 |
| C | -3.53415 | -13.5299 | -3.73488 |
| N | -3.68683 | -14.6378 | -4.05739 |
| C | -12.6064 | 0.621522 | 5.160854 |
| N | -13.6934 | 0.860039 | 5.501813 |
| C | -1.95864 | 13.90089 | -3.43132 |
| N | -1.95538 | 15.04493 | -3.64536 |
| C | 14.995 | -0.56085 | 3.149314 |
| N | 16.08295 | -0.796 | 3.489419 |

**Table S2:** Cartesian coordinates of **A1D1**

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | -2.5389 | -0.46343 | -0.8724 |
| C | -1.94146 | 0.751126 | -1.20987 |
| C | -2.69551 | 1.939896 | -1.0731 |
| C | -4.02666 | 1.912735 | -0.69985 |
| C | -4.64301 | 0.682163 | -0.42176 |
| C | -3.87647 | -0.4933 | -0.50215 |
| H | -1.9739 | -1.39081 | -0.89286 |
| H | -4.58672 | 2.839248 | -0.5796 |
| C | -0.51091 | 2.570181 | -1.56001 |
| C | 0.482103 | 3.462716 | -1.96444 |
| C | 0.200758 | 4.820343 | -2.03934 |
| C | -1.08117 | 5.327205 | -1.76108 |

| | | | |
|---|---|---|---|
| C | -2.09746 | 4.42172 | -1.41675 |
| C | -1.81247 | 3.071264 | -1.32771 |
| H | 1.478249 | 3.115969 | -2.22401 |
| H | -3.11263 | 4.785008 | -1.26144 |
| C | -0.54574 | 1.10201 | -1.50919 |
| C | 0.982223 | -3.5799 | -3.55772 |
| C | 2.021007 | -2.86918 | -2.93618 |
| C | 1.754962 | -1.65366 | -2.33211 |
| C | 0.451161 | -1.10804 | -2.3042 |
| C | -0.56701 | -1.78493 | -2.97599 |
| C | -0.3038 | -3.01157 | -3.57161 |
| H | 3.037436 | -3.25932 | -2.96958 |
| H | -1.56867 | -1.36992 | -3.04366 |
| C | 2.660539 | -0.69713 | -1.70787 |
| C | 4.006829 | -0.80528 | -1.41299 |
| C | 4.65175 | 0.23504 | -0.7247 |
| C | 3.89644 | 1.350444 | -0.32355 |
| C | 2.542879 | 1.453615 | -0.61483 |
| C | 1.915196 | 0.451527 | -1.35432 |
| H | 4.559346 | -1.70724 | -1.6734 |
| H | 4.384743 | 2.166219 | 0.201699 |
| H | 1.991511 | 2.319176 | -0.25982 |
| C | 0.504131 | 0.231873 | -1.70281 |
| H | -4.34622 | -1.45154 | -0.29773 |
| C | -1.35562 | 6.761569 | -1.83243 |
| C | -2.26553 | 9.038661 | -1.37614 |
| C | -1.41273 | 9.006203 | -2.43768 |
| C | -6.0558 | 0.624545 | -0.05772 |
| C | -8.52114 | 1.023835 | 0.036979 |
| C | -8.08077 | 0.045659 | 0.906622 |
| C | 1.237169 | -4.87733 | -4.18209 |
| C | 0.729588 | -5.41563 | -5.34627 |
| S | 2.354339 | -5.98441 | -3.41476 |
| C | 1.251956 | -6.71717 | -5.60391 |
| C | 2.131395 | -7.15537 | -4.66028 |
| H | 0.979119 | -7.29606 | -6.48251 |
| C | 6.081931 | 0.158589 | -0.43869 |
| C | 8.526832 | -0.35045 | -0.58276 |
| C | 8.157628 | 0.29209 | 0.583224 |
| H | 1.000016 | 5.509068 | -2.2995 |
| H | -1.11937 | -3.5537 | -4.04269 |
| S | -7.17647 | 1.690174 | -0.84989 |
| S | -2.45136 | 7.476876 | -0.66929 |
| S | 7.133304 | -0.57954 | -1.60615 |
| C | 6.784996 | 0.589419 | 0.680815 |
| C | -6.6932 | -0.1921 | 0.867501 |
| C | -0.88248 | 7.711623 | -2.71316 |
| H | -8.74784 | -0.46976 | 1.594492 |

| | | | |
|---|---|---|---|
| H | -1.16499 | 9.880935 | -3.03348 |
| H | 8.870289 | 0.558846 | 1.360444 |
| C | -9.83251 | 1.542593 | -0.16612 |
| C | -11.0443 | 0.992224 | 0.113394 |
| H | -9.90047 | 2.570904 | -0.53246 |
| C | 9.808203 | -0.75502 | -1.05433 |
| C | 10.98687 | -0.93836 | -0.39942 |
| H | 9.90615 | -0.86638 | -2.13817 |
| C | -13.2457 | 1.101838 | 0.884562 |
| C | -12.7938 | -0.16692 | 1.16529 |
| C | -13.7267 | -0.90125 | 1.974608 |
| C | -14.8848 | -0.11763 | 2.212389 |
| S | -14.8069 | 1.477828 | 1.481859 |
| C | 15.09239 | -0.22595 | 1.343465 |
| C | 13.30754 | -0.74759 | -0.22921 |
| C | 12.81406 | -0.67458 | 1.052572 |
| C | -12.2305 | 1.895998 | 0.180629 |
| C | -11.4999 | -0.34594 | 0.492088 |
| C | 12.23832 | -0.95907 | -1.21303 |
| C | 11.38515 | -1.0182 | 1.005382 |
| C | 13.84005 | -0.33824 | 2.001507 |
| S | 14.99526 | -0.50155 | -0.38836 |
| C | -13.6342 | -2.15269 | 2.600285 |
| H | -12.7523 | -2.77337 | 2.493207 |
| C | -15.9422 | -0.58069 | 2.987386 |
| H | -16.8291 | 0.022202 | 3.157338 |
| C | -14.6788 | -2.61191 | 3.378195 |
| C | -15.8393 | -1.83431 | 3.563484 |
| C | 16.25679 | 0.110269 | 2.024578 |
| H | 17.21235 | 0.184031 | 1.513721 |
| C | 13.78367 | -0.03434 | 3.368856 |
| H | 12.84677 | -0.05783 | 3.913057 |
| C | 14.93681 | 0.309916 | 4.046561 |
| C | 16.1775 | 0.369618 | 3.381065 |
| C | 0.035448 | 7.45908 | -3.86764 |
| H | 1.087447 | 7.615487 | -3.59577 |
| H | -0.05527 | 6.436474 | -4.24773 |
| H | -0.18722 | 8.148075 | -4.6893 |
| C | 6.191804 | 1.238968 | 1.890935 |
| H | 6.155307 | 2.331152 | 1.793711 |
| H | 5.170893 | 0.891417 | 2.078101 |
| H | 6.794961 | 1.012938 | 2.775692 |
| C | -6.02211 | -1.18018 | 1.767734 |
| H | -6.0114 | -2.18509 | 1.327496 |
| H | -4.98491 | -0.90187 | 1.978453 |
| H | -6.55777 | -1.25242 | 2.71969 |
| C | -0.2153 | -4.7387 | -6.28878 |
| H | -1.26095 | -4.99385 | -6.07295 |

| | | | |
|---|---|---|---|
| H | -0.12939 | -3.64837 | -6.2432 |
| H | -0.01605 | -5.05251 | -7.31899 |
| O | -12.3104 | 3.044485 | -0.20673 |
| O | 12.33846 | -1.0677 | -2.41866 |
| C | 10.64755 | -1.59454 | 2.012973 |
| C | -10.9772 | -1.5327 | 0.035556 |
| C | 11.14817 | -1.83202 | 3.325651 |
| N | 11.51533 | -2.05882 | 4.406797 |
| C | 9.371317 | -2.18638 | 1.777647 |
| N | 8.342525 | -2.7053 | 1.613749 |
| C | -9.87499 | -1.5907 | -0.86861 |
| N | -9.0037 | -1.69036 | -1.63382 |
| C | -11.5874 | -2.80097 | 0.256925 |
| N | -12.0536 | -3.85833 | 0.39765 |
| Cl | 17.62683 | 0.78749 | 4.235345 |
| Cl | 14.82507 | 0.677964 | 5.739699 |
| Cl | -17.1545 | -2.41299 | 4.533329 |
| Cl | -14.5309 | -4.16895 | 4.132044 |
| H | 2.663328 | -8.09767 | -4.61928 |
| H | -2.79701 | 9.886682 | -0.96265 |

**Table S3:** Cartesian coordinates of **A1D2**

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | -2.56361 | -0.44747 | -1.15206 |
| C | -1.95206 | 0.768691 | -1.45656 |
| C | -2.69481 | 1.962003 | -1.29764 |
| C | -4.02862 | 1.939701 | -0.93393 |
| C | -4.65737 | 0.709093 | -0.68532 |
| C | -3.90304 | -0.47235 | -0.78874 |
| H | -2.00796 | -1.37982 | -1.19095 |
| H | -4.58045 | 2.868537 | -0.79514 |
| C | -0.49934 | 2.580099 | -1.74916 |
| C | 0.507621 | 3.471595 | -2.12016 |
| C | 0.241885 | 4.833604 | -2.1622 |
| C | -1.03721 | 5.347819 | -1.88376 |
| C | -2.0671 | 4.444885 | -1.57435 |
| C | -1.79759 | 3.089645 | -1.51717 |
| H | 1.502663 | 3.120852 | -2.37862 |
| H | -3.08021 | 4.814277 | -1.42033 |
| C | -0.55005 | 1.112022 | -1.73451 |
| C | 0.955275 | -3.54302 | -3.86188 |
| C | 1.993599 | -2.85527 | -3.21424 |
| C | 1.732579 | -1.64931 | -2.5895 |
| C | 0.434317 | -1.09031 | -2.56723 |
| C | -0.58227 | -1.74287 | -3.26506 |
| C | -0.32452 | -2.96063 | -3.8807 |
| H | 3.006043 | -3.25596 | -3.2423 |
| H | -1.57858 | -1.31593 | -3.33741 |

| | | | |
|---|---|---|---|
| C | 2.639146 | -0.71669 | -1.93141 |
| C | 3.97904 | -0.84659 | -1.61757 |
| C | 4.622176 | 0.168949 | -0.8911 |
| C | 3.872414 | 1.282479 | -0.4746 |
| C | 2.525935 | 1.408747 | -0.78807 |
| C | 1.900807 | 0.431708 | -1.56237 |
| H | 4.526025 | -1.74832 | -1.89002 |
| H | 4.359963 | 2.078654 | 0.080253 |
| H | 1.977112 | 2.27115 | -0.42174 |
| C | 0.492866 | 0.23507 | -1.93586 |
| H | -4.38323 | -1.43019 | -0.60856 |
| C | -1.29354 | 6.786604 | -1.91888 |
| C | -2.18452 | 9.061044 | -1.41433 |
| C | -1.30714 | 9.049302 | -2.45611 |
| C | -6.07054 | 0.658248 | -0.32307 |
| C | -8.53137 | 1.076311 | -0.21553 |
| C | -8.09435 | 0.084848 | 0.644367 |
| C | 1.204359 | -4.83172 | -4.50602 |
| C | 0.703433 | -5.34564 | -5.68417 |
| S | 2.302475 | -5.9626 | -3.74584 |
| C | 1.215593 | -6.64789 | -5.95807 |
| C | 2.080908 | -7.11038 | -5.01291 |
| H | 0.94588 | -7.20973 | -6.8486 |
| C | 6.044793 | 0.067428 | -0.57944 |
| C | 8.483721 | -0.47851 | -0.67807 |
| C | 8.095467 | 0.144004 | 0.495664 |
| H | 1.05118 | 5.519727 | -2.39643 |
| H | -1.13994 | -3.48522 | -4.37149 |
| S | -7.18264 | 1.738816 | -1.10218 |
| S | -2.40818 | 7.481134 | -0.76111 |
| S | 7.108818 | -0.65991 | -1.73886 |
| C | 6.728846 | 0.462754 | 0.567531 |
| C | -6.71138 | -0.16389 | 0.597753 |
| C | -0.78708 | 7.756714 | -2.75862 |
| H | -8.76144 | -0.42911 | 1.333164 |
| H | -1.03442 | 9.93812 | -3.01922 |
| H | 8.792655 | 0.382725 | 1.295399 |
| C | -9.8321 | 1.615061 | -0.40423 |
| C | -11.0547 | 1.106555 | -0.0781 |
| H | -9.88462 | 2.632593 | -0.80184 |
| C | 9.764991 | -0.87985 | -1.1389 |
| C | 10.95656 | -1.03762 | -0.49145 |
| H | 9.859372 | -1.01119 | -2.22094 |
| C | -13.238 | 1.299745 | 0.734625 |
| C | -12.8152 | 0.027927 | 1.037277 |
| C | -13.7518 | -0.65427 | 1.882018 |
| C | -14.8809 | 0.170426 | 2.124219 |
| S | -14.7738 | 1.73679 | 1.352751 |

| | | | |
|---|---|---|---|
| C | 15.08904 | -0.2931 | 1.171269 |
| C | 13.28073 | -0.82806 | -0.35879 |
| C | 12.80648 | -0.74884 | 0.927596 |
| C | -12.2075 | 2.047716 | -0.00923 |
| C | -11.5362 | -0.20565 | 0.346846 |
| C | 12.19148 | -1.05389 | -1.32501 |
| C | 11.37358 | -1.09295 | 0.906305 |
| C | 13.84906 | -0.40805 | 1.853252 |
| S | 14.96349 | -0.57753 | -0.54943 |
| C | -13.6727 | -1.88636 | 2.552234 |
| H | -12.7964 | -2.52046 | 2.483923 |
| C | -15.9444 | -0.24913 | 2.921604 |
| H | -16.8341 | 0.355758 | 3.067223 |
| C | -14.7122 | -2.28506 | 3.358198 |
| C | -15.8571 | -1.4843 | 3.521874 |
| C | 16.27135 | 0.033733 | 1.833814 |
| H | 17.22766 | 0.073236 | 1.321313 |
| C | 13.81427 | -0.08824 | 3.220215 |
| H | 12.88778 | -0.06917 | 3.782574 |
| C | 14.97934 | 0.251002 | 3.86618 |
| C | 16.20909 | 0.286963 | 3.184261 |
| C | 0.156845 | 7.528051 | -3.89706 |
| H | 1.204268 | 7.643548 | -3.58931 |
| H | 0.050585 | 6.52495 | -4.32269 |
| H | -0.02351 | 8.257115 | -4.69404 |
| C | 6.117041 | 1.094687 | 1.777494 |
| H | 6.083822 | 2.188176 | 1.696319 |
| H | 5.092751 | 0.745883 | 1.942294 |
| H | 6.705392 | 0.853586 | 2.668074 |
| C | -6.04364 | -1.16624 | 1.484327 |
| H | -6.03856 | -2.16508 | 1.030664 |
| H | -5.00494 | -0.8954 | 1.696981 |
| H | -6.57827 | -1.24828 | 2.435938 |
| C | -0.22512 | -4.64351 | -6.62446 |
| H | -1.27518 | -4.89298 | -6.42401 |
| H | -0.12989 | -3.55495 | -6.55858 |
| H | -0.01782 | -4.94083 | -7.65795 |
| O | -12.2658 | 3.188546 | -0.4193 |
| O | 12.27953 | -1.17023 | -2.52999 |
| C | 10.65932 | -1.64894 | 1.940883 |
| C | -11.0623 | -1.42307 | -0.07979 |
| C | 11.18471 | -1.84033 | 3.251447 |
| N | 11.57694 | -2.02336 | 4.332096 |
| C | 9.384821 | -2.25602 | 1.742621 |
| N | 8.357233 | -2.78464 | 1.605565 |
| C | -9.98389 | -1.54497 | -1.00533 |
| N | -9.12899 | -1.68529 | -1.78229 |
| C | -11.7078 | -2.66005 | 0.209891 |

| | | | |
|---|---|---|---|
| N | -12.213 | -3.68832 | 0.416359 |
| N | 14.8572 | 0.731504 | 5.246807 |
| O | 15.60794 | 1.629615 | 5.587002 |
| O | 13.98566 | 0.235093 | 5.937292 |
| N | 17.48636 | 0.461679 | 3.884876 |
| O | 18.34726 | 1.108817 | 3.315316 |
| O | 17.6105 | -0.10236 | 4.956266 |
| N | -17.0542 | -1.96726 | 4.219166 |
| O | -17.7108 | -1.14328 | 4.831406 |
| O | -17.3331 | -3.14533 | 4.08954 |
| N | -14.4979 | -3.49308 | 4.164608 |
| O | -14.9173 | -3.4745 | 5.308563 |
| O | -13.8718 | -4.4029 | 3.651828 |
| H | 2.602758 | -8.05869 | -4.98188 |
| H | -2.71495 | 9.903148 | -0.98765 |

**Table S4:** Cartesian coordinates of **A1D3**

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | 2.527374 | 0.506543 | 1.279112 |
| C | 1.918579 | 1.739812 | 1.048785 |
| C | 2.642089 | 2.735669 | 0.351786 |
| C | 3.956444 | 2.539294 | -0.03062 |
| C | 4.586286 | 1.317106 | 0.255452 |
| C | 3.848657 | 0.310405 | 0.902817 |
| H | 1.985414 | -0.30787 | 1.750803 |
| H | 4.490608 | 3.308312 | -0.58758 |
| C | 0.465888 | 3.51685 | 0.597697 |
| C | -0.52986 | 4.493807 | 0.600652 |
| C | -0.27465 | 5.739841 | 0.043477 |
| C | 0.984103 | 6.067439 | -0.49107 |
| C | 2.004557 | 5.104695 | -0.43891 |
| C | 1.746257 | 3.859422 | 0.105528 |
| H | -1.50788 | 4.298626 | 1.032322 |
| H | 3.004235 | 5.358275 | -0.78979 |
| C | 0.528269 | 2.185299 | 1.214045 |
| C | -0.85892 | -1.09674 | 5.182457 |
| C | -1.92622 | -0.74807 | 4.339376 |
| C | -1.69832 | 0.072425 | 3.249391 |
| C | -0.40723 | 0.561493 | 2.94585 |
| C | 0.639886 | 0.264791 | 3.818459 |
| C | 0.415 | -0.56986 | 4.904992 |
| H | -2.93334 | -1.09233 | 4.571345 |
| H | 1.633248 | 0.676911 | 3.664253 |
| C | -2.63522 | 0.63871 | 2.286354 |
| C | -3.98078 | 0.383623 | 2.095227 |
| C | -4.6557 | 0.992217 | 1.025297 |
| C | -3.9344 | 1.831118 | 0.158185 |
| C | -2.58236 | 2.082595 | 0.349238 |

| | | | |
|---|---|---|---|
| C | -1.9224 | 1.522043 | 1.442552 |
| H | -4.50645 | -0.32155 | 2.737532 |
| H | -4.44892 | 2.31515 | -0.6674 |
| H | -2.05553 | 2.713366 | -0.36124 |
| C | -0.5 | 1.492779 | 1.813925 |
| H | 4.329086 | -0.63493 | 1.138682 |
| C | 1.228908 | 7.38246 | -1.08239 |
| C | 2.056292 | 9.215907 | -2.55744 |
| C | 1.259885 | 9.66099 | -1.54605 |
| C | 5.981446 | 1.094524 | -0.11135 |
| C | 8.429267 | 1.399352 | -0.51603 |
| C | 7.975376 | 0.12268 | -0.78053 |
| C | -1.07021 | -1.98228 | 6.326346 |
| C | -0.51071 | -1.94593 | 7.586356 |
| S | -2.1894 | -3.32009 | 6.17618 |
| C | -0.99407 | -3.00029 | 8.415638 |
| C | -1.8958 | -3.81585 | 7.801637 |
| H | -0.67735 | -3.12788 | 9.447559 |
| C | -6.08137 | 0.752521 | 0.814482 |
| C | -8.51117 | 0.295052 | 1.17962 |
| C | -8.14203 | 0.32065 | -0.15116 |
| H | -1.07714 | 6.47131 | 0.001195 |
| H | 1.251044 | -0.83796 | 5.54549 |
| S | 7.110472 | 2.411569 | 0.006497 |
| S | 2.246347 | 7.502707 | -2.50188 |
| S | -7.13027 | 0.621992 | 2.191819 |
| C | -6.77687 | 0.582963 | -0.3762 |
| C | 6.597315 | -0.06679 | -0.56053 |
| C | 0.777219 | 8.625846 | -0.69245 |
| H | 8.6199 | -0.65817 | -1.17842 |
| H | 1.021568 | 10.70982 | -1.38899 |
| H | -8.85161 | 0.16349 | -0.96051 |
| C | 9.735852 | 1.947098 | -0.67528 |
| C | 10.94194 | 1.319889 | -0.68505 |
| H | 9.798074 | 3.014485 | -0.90503 |
| C | -9.7956 | 0.118264 | 1.771837 |
| C | -10.9266 | -0.44694 | 1.271111 |
| H | -9.94313 | 0.573653 | 2.755512 |
| C | 13.0976 | 0.971222 | -1.51366 |
| C | 12.65548 | -0.24297 | -1.0418 |
| C | 13.55976 | -1.30809 | -1.37153 |
| C | 14.68914 | -0.79498 | -2.05639 |
| S | 14.61868 | 0.941696 | -2.30243 |
| C | -14.9323 | -1.05482 | -0.72601 |
| C | -13.2382 | -0.53409 | 0.947766 |
| C | -12.6636 | -1.11052 | -0.16152 |
| C | 12.10692 | 2.033121 | -1.28915 |
| C | 11.39978 | -0.01989 | -0.31347 |

| | | | |
|---|---|---|---|
| C | -12.2266 | -0.12433 | 1.931296 |
| C | -11.2284 | -1.27691 | 0.104399 |
| C | -13.6344 | -1.39967 | -1.1788 |
| S | -14.9426 | -0.3684 | 0.889465 |
| C | 13.45695 | -2.6991 | -1.21687 |
| H | 12.5751 | -3.14198 | -0.76861 |
| C | 15.72161 | -1.62157 | -2.4929 |
| H | 16.59975 | -1.20906 | -2.98142 |
| C | 14.46985 | -3.52752 | -1.66297 |
| C | 15.623 | -2.9858 | -2.27736 |
| C | -16.0613 | -1.2341 | -1.52215 |
| H | -17.0543 | -1.00407 | -1.14666 |
| C | -13.4947 | -1.84578 | -2.50236 |
| H | -12.5146 | -2.04138 | -2.92209 |
| C | -14.6088 | -2.00527 | -3.30519 |
| C | -15.9026 | -1.7302 | -2.80484 |
| C | -0.07447 | 8.917366 | 0.50327 |
| H | -1.14288 | 8.929829 | 0.251394 |
| H | 0.065265 | 8.176724 | 1.297074 |
| H | 0.168578 | 9.903771 | 0.912347 |
| C | -6.18141 | 0.610038 | -1.74822 |
| H | -6.1885 | 1.620081 | -2.17658 |
| H | -5.14372 | 0.262021 | -1.74686 |
| H | -6.7557 | -0.03183 | -2.42336 |
| C | 5.913354 | -1.36599 | -0.84611 |
| H | 5.9205 | -2.02941 | 0.0277 |
| H | 4.869753 | -1.22138 | -1.14171 |
| H | 6.427524 | -1.89503 | -1.65485 |
| C | 0.451408 | -0.91728 | 8.091899 |
| H | 1.494624 | -1.23125 | 7.956852 |
| H | 0.330815 | 0.043336 | 7.580752 |
| H | 0.303996 | -0.75247 | 9.164534 |
| O | 12.18678 | 3.209748 | -1.5793 |
| O | -12.3989 | 0.408333 | 3.009036 |
| C | -10.4074 | -2.24316 | -0.42639 |
| C | 10.91959 | -0.77447 | 0.730046 |
| C | -10.8176 | -3.17388 | -1.42487 |
| N | -11.1005 | -3.96846 | -2.22717 |
| C | -9.11801 | -2.53057 | 0.112931 |
| N | -8.07597 | -2.82028 | 0.542743 |
| C | 9.854631 | -0.33391 | 1.571767 |
| N | 9.01496 | -0.00619 | 2.308051 |
| C | 11.5407 | -1.97052 | 1.194316 |
| N | 12.01674 | -2.94291 | 1.622341 |
| H | -2.40784 | -4.68062 | 8.204899 |
| H | 2.545193 | 9.789651 | -3.33482 |
| C | 16.8067 | -3.84482 | -2.57141 |
| O | 17.22389 | -4.69692 | -1.82249 |

| | | | |
|---|---|---|---|
| O | 17.38866 | -3.50547 | -3.72519 |
| C | 14.26095 | -5.00303 | -1.63071 |
| O | 14.62942 | -5.76012 | -2.49971 |
| O | 13.56278 | -5.37672 | -0.55541 |
| C | -17.1145 | -2.09684 | -3.59325 |
| O | -17.2134 | -3.10814 | -4.24824 |
| O | -18.0961 | -1.20561 | -3.42986 |
| C | -14.4158 | -2.31568 | -4.75065 |
| O | -15.0581 | -1.81145 | -5.64329 |
| O | -13.4072 | -3.16989 | -4.93924 |
| C | -13.0989 | -3.45937 | -6.30465 |
| H | -12.8489 | -2.54201 | -6.84469 |
| H | -12.2438 | -4.13394 | -6.28205 |
| H | -13.9511 | -3.93929 | -6.79343 |
| C | -19.3232 | -1.52768 | -4.09063 |
| H | -19.7201 | -2.47634 | -3.71896 |
| H | -20.0093 | -0.71223 | -3.86501 |
| H | -19.164 | -1.6063 | -5.16924 |
| C | 18.58185 | -4.2297 | -4.03722 |
| H | 18.93746 | -3.82978 | -4.9862 |
| H | 19.33297 | -4.08576 | -3.25587 |
| H | 18.36496 | -5.29705 | -4.13056 |
| C | 13.24105 | -6.76776 | -0.48892 |
| H | 12.67525 | -6.8999 | 0.432596 |
| H | 12.64027 | -7.06383 | -1.35339 |
| H | 14.15349 | -7.3695 | -0.4665 |

**Table S5:** Cartesian coordinates of **A1D4**

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | -2.46393 | -0.58218 | -1.04874 |
| C | -1.89959 | 0.657223 | -1.35048 |
| C | -2.68264 | 1.822153 | -1.17202 |
| C | -4.00658 | 1.749474 | -0.78137 |
| C | -4.58871 | 0.495697 | -0.53288 |
| C | -3.79555 | -0.65772 | -0.66429 |
| H | -1.87753 | -1.49451 | -1.10521 |
| H | -4.58549 | 2.658099 | -0.62092 |
| C | -0.52023 | 2.522595 | -1.6571 |
| C | 0.447492 | 3.449233 | -2.04598 |
| C | 0.129487 | 4.79972 | -2.0924 |
| C | -1.16496 | 5.265622 | -1.80016 |
| C | -2.15443 | 4.326871 | -1.4664 |
| C | -1.83291 | 2.98307 | -1.40556 |
| H | 1.451409 | 3.133672 | -2.31548 |
| H | -3.17803 | 4.659807 | -1.29889 |
| C | -0.51487 | 1.05358 | -1.64296 |
| C | 1.174152 | -3.53706 | -3.77381 |
| C | 2.185965 | -2.80556 | -3.13134 |

| | | | |
|---|---|---|---|
| C | 1.8779 | -1.61015 | -2.50774 |
| C | 0.557324 | -1.10606 | -2.48121 |
| C | -0.43412 | -1.8008 | -3.17436 |
| C | -0.12854 | -3.00804 | -3.78908 |
| H | 3.214045 | -3.16398 | -3.16213 |
| H | -1.44724 | -1.41452 | -3.24303 |
| C | 2.747297 | -0.64003 | -1.8532 |
| C | 4.092492 | -0.71403 | -1.5409 |
| C | 4.69141 | 0.324899 | -0.81087 |
| C | 3.896436 | 1.406037 | -0.39329 |
| C | 2.546241 | 1.477462 | -0.70713 |
| C | 1.961974 | 0.476172 | -1.482 |
| H | 4.67778 | -1.59083 | -1.81498 |
| H | 4.351044 | 2.22022 | 0.16379 |
| H | 1.963816 | 2.316854 | -0.33964 |
| C | 0.562067 | 0.220477 | -1.85098 |
| H | -4.23809 | -1.63392 | -0.48778 |
| C | -1.47985 | 6.692559 | -1.84851 |
| C | -2.45318 | 8.935584 | -1.35674 |
| C | -1.60503 | 8.94257 | -2.42255 |
| C | -5.99146 | 0.397195 | -0.1423 |
| C | -8.45637 | 0.769516 | 0.044587 |
| C | -7.9812 | -0.24753 | 0.852771 |
| C | 1.473074 | -4.81547 | -4.41726 |
| C | 0.98553 | -5.35243 | -5.59076 |
| S | 2.624065 | -5.89743 | -3.66378 |
| C | 1.550059 | -6.63245 | -5.86638 |
| C | 2.441335 | -7.0561 | -4.92731 |
| H | 1.29726 | -7.20683 | -6.75387 |
| C | 6.11532 | 0.282834 | -0.48832 |
| C | 8.57896 | -0.12565 | -0.5778 |
| C | 8.14746 | 0.430546 | 0.6116 |
| H | 0.908277 | 5.515634 | -2.34074 |
| H | -0.92359 | -3.56652 | -4.27569 |
| S | -7.14226 | 1.484776 | -0.85294 |
| S | -2.59007 | 7.359521 | -0.67078 |
| S | 7.230232 | -0.34509 | -1.66145 |
| C | 6.763545 | 0.674223 | 0.677963 |
| C | -6.59599 | -0.4708 | 0.761376 |
| C | -1.03881 | 7.667801 | -2.71839 |
| H | -8.61999 | -0.79941 | 1.538966 |
| H | -1.38537 | 9.832185 | -3.00717 |
| H | 8.825801 | 0.675408 | 1.425979 |
| C | -9.76599 | 1.304578 | -0.08537 |
| C | -10.978 | 0.788141 | 0.265892 |
| H | -9.83346 | 2.332948 | -0.45186 |
| C | 9.897932 | -0.44181 | -1.00795 |
| C | 11.02949 | -0.65363 | -0.27986 |

| | | | |
|---|---|---|---|
| H | 10.07373 | -0.43684 | -2.08733 |
| C | -13.1323 | 0.968442 | 1.152969 |
| C | -12.7074 | -0.31239 | 1.411424 |
| C | -13.6179 | -1.00913 | 2.27651 |
| C | -14.7349 | -0.18263 | 2.573693 |
| S | -14.6426 | 1.401833 | 1.832989 |
| C | 14.92461 | -0.0294 | 1.917647 |
| C | 13.31767 | -0.41538 | 0.131253 |
| C | 12.70753 | -0.52916 | 1.357213 |
| C | -12.1248 | 1.730435 | 0.394691 |
| C | -11.4523 | -0.53226 | 0.67351 |
| C | 12.34488 | -0.53189 | -0.97022 |
| C | 11.3015 | -0.90077 | 1.135225 |
| C | 13.62397 | -0.2763 | 2.433237 |
| S | 14.99738 | -0.08359 | 0.167884 |
| C | -13.5307 | -2.25905 | 2.906491 |
| H | -12.6765 | -2.90775 | 2.751962 |
| C | -15.7677 | -0.60016 | 3.407027 |
| H | -16.6208 | 0.038887 | 3.613376 |
| C | -14.5473 | -2.67776 | 3.749257 |
| C | -15.6786 | -1.85411 | 3.992061 |
| C | 16.00661 | 0.261309 | 2.742625 |
| H | 16.99806 | 0.432947 | 2.334316 |
| C | 13.42106 | -0.15241 | 3.815167 |
| H | 12.43814 | -0.28377 | 4.252973 |
| C | 14.48962 | 0.148876 | 4.643248 |
| C | 15.79184 | 0.343641 | 4.110371 |
| C | -0.1204 | 7.458238 | -3.88118 |
| H | 0.927457 | 7.647769 | -3.61438 |
| H | -0.17875 | 6.437119 | -4.2714 |
| H | -0.3719 | 8.147536 | -4.69426 |
| C | 6.107287 | 1.235321 | 1.899601 |
| H | 6.038948 | 2.329529 | 1.861194 |
| H | 5.092405 | 0.846855 | 2.029558 |
| H | 6.686314 | 0.978718 | 2.792062 |
| C | -5.89062 | -1.49427 | 1.593034 |
| H | -5.85026 | -2.46735 | 1.087984 |
| H | -4.86184 | -1.19782 | 1.819629 |
| H | -6.41919 | -1.64522 | 2.53948 |
| C | 0.021931 | -4.69237 | -6.52633 |
| H | -1.01625 | -4.97887 | -6.31391 |
| H | 0.077294 | -3.60056 | -6.4693 |
| H | 0.230197 | -4.9895 | -7.55967 |
| O | -12.1922 | 2.881436 | 0.014775 |
| O | 12.55904 | -0.4801 | -2.16377 |
| C | 10.50811 | -1.6223 | 1.994244 |
| C | -10.9929 | -1.73742 | 0.198018 |
| C | 10.92377 | -2.03021 | 3.294423 |

| | | | |
|---|---|---|---|
| N | 11.22672 | -2.39886 | 4.356171 |
| C | 9.264574 | -2.19574 | 1.594158 |
| N | 8.261532 | -2.70833 | 1.302229 |
| C | -9.9448 | -1.83203 | -0.76467 |
| N | -9.11511 | -1.94954 | -1.57217 |
| C | -11.6316 | -2.9825 | 0.464854 |
| N | -12.1312 | -4.01812 | 0.646292 |
| H | 3.003565 | -7.9811 | -4.89925 |
| H | -3.00637 | 9.762153 | -0.92862 |
| C | -14.4498 | -3.95241 | 4.389781 |
| N | -14.374 | -4.98641 | 4.914629 |
| C | -16.7217 | -2.30615 | 4.857617 |
| N | -17.5715 | -2.67178 | 5.561148 |
| C | 16.88423 | 0.644686 | 4.980984 |
| N | 17.77303 | 0.88942 | 5.688728 |
| C | 14.27221 | 0.275204 | 6.050927 |
| N | 14.09603 | 0.38139 | 7.1946 |

**Table S6:** Cartesian coordinates of **A1D5**

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | -2.51489 | -0.63491 | -0.52066 |
| C | -1.94775 | 0.570114 | -0.93611 |
| C | -2.73346 | 1.74473 | -0.88304 |
| C | -4.06539 | 1.707686 | -0.51426 |
| C | -4.65062 | 0.482759 | -0.15493 |
| C | -3.85297 | -0.67475 | -0.15294 |
| H | -1.92583 | -1.54677 | -0.48007 |
| H | -4.6498 | 2.625315 | -0.45945 |
| C | -0.56299 | 2.399871 | -1.39848 |
| C | 0.409805 | 3.288715 | -1.8564 |
| C | 0.091653 | 4.628925 | -2.03155 |
| C | -1.20656 | 5.117712 | -1.80036 |
| C | -2.20013 | 4.212195 | -1.39569 |
| C | -1.87923 | 2.879768 | -1.2095 |
| H | 1.417964 | 2.9515 | -2.08031 |
| H | -3.22573 | 4.557699 | -1.2716 |
| C | -0.55978 | 0.937839 | -1.24981 |
| C | 1.104632 | -3.81034 | -3.01445 |
| C | 2.120786 | -3.03786 | -2.42974 |
| C | 1.818216 | -1.7988 | -1.89444 |
| C | 0.499628 | -1.28944 | -1.90098 |
| C | -0.49763 | -2.03211 | -2.53361 |
| C | -0.19739 | -3.28147 | -3.06032 |
| H | 3.148183 | -3.39957 | -2.44048 |
| H | -1.51045 | -1.6495 | -2.62394 |
| C | 2.694394 | -0.78245 | -1.32511 |
| C | 4.041841 | -0.83438 | -1.0204 |
| C | 4.653545 | 0.262461 | -0.39277 |

| | | | |
|---|---|---|---|
| C | 3.866121 | 1.378379 | -0.06005 |
| C | 2.512087 | 1.426601 | -0.36399 |
| C | 1.916384 | 0.36464 | -1.04387 |
| H | 4.620732 | -1.73388 | -1.22546 |
| H | 4.328813 | 2.235596 | 0.421505 |
| H | 1.935162 | 2.297048 | -0.06552 |
| C | 0.513568 | 0.085386 | -1.38268 |
| H | -4.29799 | -1.6283 | 0.118321 |
| C | -1.52019 | 6.533998 | -1.98488 |
| C | -2.49217 | 8.815024 | -1.71557 |
| C | -1.63945 | 8.718325 | -2.77314 |
| C | -6.06265 | 0.413517 | 0.208726 |
| C | -8.53618 | 0.764956 | 0.27984 |
| C | -8.07698 | -0.15443 | 1.202478 |
| C | 1.398329 | -5.12894 | -3.57372 |
| C | 0.906999 | -5.73433 | -4.71121 |
| S | 2.548227 | -6.16624 | -2.75786 |
| C | 1.4673 | -7.03033 | -4.91002 |
| C | 2.359185 | -7.399 | -3.94902 |
| H | 1.211605 | -7.65596 | -5.76127 |
| C | 6.084208 | 0.241507 | -0.09878 |
| C | 8.542498 | -0.20055 | -0.21048 |
| C | 8.147484 | 0.472111 | 0.930233 |
| H | 0.873103 | 5.319893 | -2.33673 |
| H | -0.9952 | -3.87245 | -3.50203 |
| S | -7.2044 | 1.411975 | -0.64003 |
| S | -2.63445 | 7.311806 | -0.8816 |
| S | 7.163217 | -0.50624 | -1.2333 |
| C | 6.766389 | 0.733909 | 1.008008 |
| C | -6.68445 | -0.36419 | 1.177178 |
| C | -1.07367 | 7.420508 | -2.94229 |
| H | -8.73057 | -0.63598 | 1.92649 |
| H | -1.41681 | 9.547326 | -3.43993 |
| H | 8.84757 | 0.786154 | 1.701338 |
| C | -9.85844 | 1.245788 | 0.053612 |
| C | -11.0569 | 0.669865 | 0.339414 |
| H | -9.95018 | 2.262471 | -0.33928 |
| C | 9.836725 | -0.58293 | -0.66294 |
| C | 11.01955 | -0.71313 | -0.0016 |
| H | 9.941376 | -0.72582 | -1.74253 |
| C | -13.2673 | 0.736212 | 1.092866 |
| C | -12.7865 | -0.51727 | 1.394339 |
| C | -13.7028 | -1.26281 | 2.211405 |
| C | -14.8826 | -0.50216 | 2.430955 |
| S | -14.8381 | 1.084236 | 1.675889 |
| C | 15.11254 | 0.132127 | 1.710242 |
| C | 13.33647 | -0.46706 | 0.158476 |
| C | 12.84437 | -0.37348 | 1.439764 |

| | | | |
|---|---|---|---|
| C | -12.2658 | 1.544263 | 0.382157 |
| C | -11.4828 | -0.67418 | 0.73383 |
| C | 12.2688 | -0.72667 | -0.81713 |
| C | 11.42165 | -0.74715 | 1.404156 |
| C | 13.86355 | 0.009766 | 2.378111 |
| S | 15.01527 | -0.18888 | -0.01435 |
| C | -13.5796 | -2.50488 | 2.858453 |
| H | -12.6754 | -3.09323 | 2.756944 |
| C | -15.9337 | -0.9752 | 3.206236 |
| H | -16.8342 | -0.38775 | 3.359249 |
| C | -14.6126 | -2.979 | 3.636981 |
| C | -15.7922 | -2.22522 | 3.801219 |
| C | 16.27342 | 0.509502 | 2.372558 |
| H | 17.22214 | 0.591424 | 1.849967 |
| C | 13.80442 | 0.34604 | 3.741961 |
| H | 12.86354 | 0.313086 | 4.278363 |
| C | 14.94917 | 0.728026 | 4.406948 |
| C | 16.18383 | 0.798416 | 3.730563 |
| C | -0.15169 | 7.098695 | -4.07608 |
| H | 0.894984 | 7.316289 | -3.82653 |
| H | -0.20639 | 6.043697 | -4.36306 |
| H | -0.4026 | 7.703065 | -4.95435 |
| C | 6.142738 | 1.410846 | 2.18718 |
| H | 6.085161 | 2.498054 | 2.052201 |
| H | 5.126451 | 1.048214 | 2.370394 |
| H | 6.736769 | 1.227289 | 3.087783 |
| C | -5.9934 | -1.28247 | 2.134388 |
| H | -5.94947 | -2.30926 | 1.750375 |
| H | -4.96671 | -0.96233 | 2.337056 |
| H | -6.53536 | -1.31816 | 3.084816 |
| C | -0.05633 | -5.12889 | -5.68327 |
| H | -1.09507 | -5.39825 | -5.45185 |
| H | 0.002901 | -4.03587 | -5.69216 |
| H | 0.148451 | -5.48912 | -6.69707 |
| O | -12.3729 | 2.683286 | -0.02511 |
| O | 12.37087 | -0.86376 | -2.01952 |
| C | 10.69814 | -1.31331 | 2.427399 |
| C | -10.9305 | -1.85372 | 0.294891 |
| C | 11.20605 | -1.51614 | 3.743125 |
| N | 11.57645 | -1.71945 | 4.827759 |
| C | 9.432526 | -1.93473 | 2.21133 |
| N | 8.413581 | -2.47824 | 2.066808 |
| C | -9.81359 | -1.89863 | -0.59213 |
| N | -8.92897 | -1.99087 | -1.34274 |
| C | -11.5186 | -3.13261 | 0.515427 |
| N | -11.9647 | -4.19919 | 0.651267 |
| H | 2.918388 | -8.32256 | -3.86593 |
| H | -3.04744 | 9.679198 | -1.37284 |

| | | | |
|---|---|---|---|
| C | -16.8521 | -2.74257 | 4.610375 |
| N | -17.7121 | -3.16586 | 5.268529 |
| C | 17.35856 | 1.193142 | 4.444543 |
| N | 18.31223 | 1.513984 | 5.027211 |
| H | -14.5233 | -3.93923 | 4.135791 |
| H | 14.90737 | 0.984292 | 5.461183 |

**Table S7:** Calculated energies ($E$) and energy gap ($\Delta E$) for **A1R1** and **A1D1-A1D5.**

| Compound | HOMO-1 | LUMO+1 | $\Delta E$ | HOMO-2 | LUMO+2 | $\Delta E$ |
|---|---|---|---|---|---|---|
| **A1R** | -6.302 | -3.043 | 3.259 | -6.324 | -3.037 | 3.287 |
| **A1D1** | -6.127 | -3.058 | 3.069 | -6.148 | -2.978 | 3.17 |
| **A1D2** | -6.208 | -3.269 | 2.939 | -6.216 | -3.257 | 2.959 |
| **A1D3** | -6.124 | -3.055 | 3.069 | -6.144 | -2.984 | 3.16 |
| **A1D4** | -6.194 | -3.223 | 2.971 | -6.205 | -3.187 | 3.018 |
| **A1D5** | -6.149 | -3.087 | 3.062 | -6.167 | -3.044 | 3.123 |

$E$= energy, $\Delta E$(e$V$)= $E_{LUMO}$-$E_{HOMO}$; HOMO= highest occupied molecular orbital; LUMO= lowest unoccupied molecular orbital, MO, molecular orbital, Units in e$V$

**Table S8:** Percentages of acceptor and $\pi$-spacer for HOMOs and LUMOs of **A1R1** and **A1D1-A1D5**.

| Compounds | HOMOs (%) | | LUMOs (%) | |
|---|---|---|---|---|
| | Acceptor | $\pi$-spacer | Acceptor | $\pi$-spacer |
| **A1R** | 17.5 | 82.5 | 18.0 | 82.0 |
| **A1D1** | 3.6 | 96.4 | 47.2 | 52.8 |
| **A1D2** | 3.1 | 96.9 | 51.9 | 48.1 |
| **A1D3** | 3.4 | 96.9 | 46.9 | 53.1 |
| **A1D4** | 3.1 | 96.9 | 54.9 | 45.1 |
| **A1D5** | 3.4 | 96.9 | 43.7 | 56.3 |

**Table S9:** Wave length, excitation energy and oscillator strength of **A1R1** and **A1D1-A1D5** in solvent phase.

| Compounds | $\lambda$ (*nm*) | $E$(*eV*) | $f_{os}$ | MO contributions |
|---|---|---|---|---|
| **A1R** | 704.816 | 1.759 | 1.852 | H→L (96%), |
| | 581.567 | 2.132 | 0.546 | H-1→L (87%), H-6→L (2%), H→L+2 (3%) |
| | 575.093 | 2.156 | 0.922 | H-2→L (86%), H-5→L (2%), H→L+1 (3%) |
| | 525.468 | 2.360 | 0.989 | H→L+1 (45%), H→L+2 (47%), |
| | 524.423 | 2.364 | 0.319 | H→L+1 (46%), H→L+2 (44%), H-2→L (3%) |
| | 492.901 | 2.515 | 0.030 | H-3→L (16%), H→L+3 (81%), |
| **A1D1** | 639.753 | 1.938 | 1.705 | H→L (81%), H→L+2 (10%), H-1→L (2%) |
| | 578.204 | 2.144 | 0.033 | H→L+1 (79%), H-3→L (2%), H-2→L (6%), H-1→L+1 (6%) |
| | 562.567 | 2.204 | 0.137 | H→L+2 (72%), H-3→L+1 (4%), H-2→L+1 (5%), H-1→L (6%), H→L (5%), H→L+4 (2%) |
| | 533.151 | 2.326 | 0.577 | H-1→L (63%), H-1→L+2 (16%), H-1→L+4 (4%), H→L (5%), H→L+2 (3%) |
| | 526.651 | 2.354 | 0.073 | H-2→L (60%), H-2→L+2 (17%), H-2→L+4 (4%), H→L+1 (7%), H→L+3 (2%) |
| | 508.904 | 2.436 | 0.017 | H-1→L+1 (11%), H→L+3 (69%), H-3→L+2 (2%), H-2→L (3%), H-2→L+2 (5%) |
| **A1D2** | 665.508 | 1.863 | 1.589 | H→L (79%), H→L+1 (5%), H→L+4 (8%) |
| | 602.772 | 2.057 | 0.024 | H→L+1 (24%), H→L+2 (15%), H→L+3 (47%), H-2→L+1 (2%) |
| | 597.514 | 2.075 | 0.030 | H→L+1 (33%), H→L+2 (49%), H-1→L+2 (3%), H→L (5%) |

| | | | | |
|---|---|---|---|---|
| | 584.280 | 2.122 | 0.035 | H→L+1 (28%), H→L+2 (23%), H→L+3 (42%) |
| | 546.668 | 2.268 | 0.678 | H-2→L (12%), H-1→L (51%), H-3→L+3 (2%), H-2→L+3 (3%), H-1→L+1 (4%), H-1→L+4 (9%), H→L+4 (2%) |
| | 538.593 | 2.302 | 0.074 | H-2→L (49%), H-2→L+4 (10%), H-1→L (12%), H-2→L+1 (4%), H-1→L+3 (4%), H-1→L+4 (3%), H→L+3 (5%) |
| **A1D3** | 640.150 | 1.937 | 1.675 | H→L (81%), H→L+2 (10%), H-1→L (2%) |
| | 578.797 | 2.142 | 0.043 | H→L+1 (79%), H-3→L (2%), H-2→L (6%), H-1→L+1 (6%) |
| | 563.616 | 2.200 | 0.134 | H→L+2 (72%), H-3→L+1 (4%), H-2→L+1 (4%), H-1→L (6%), H→L (6%), H→L+4 (3%) |
| | 533.105 | 2.326 | 0.562 | H-1→L (65%), H-1→L+2 (14%), H-1→L+4 (5%), H→L (5%), H→L+2 (3%) |
| | 526.897 | 2.353 | 0.090 | H-2→L (58%), H-2→L+2 (16%), H-2→L+4 (5%), H→L+1 (6%), H→L+3 (6%) |
| | 512.904 | 2.417 | 0.015 | H→L+3 (77%), H-2→L (7%), H-1→L+1 (6%) |
| **A1D4** | 656.696 | 1.888 | 1.615 | H→L (76%), H→L+2 (11%), H-1→L (2%), H→L+1 (3%), H→L+4 (4%) |
| | 601.515 | 2.061 | 0.025 | H→L+1 (80%), H-3→L (2%), H-2→L (2%), H-1→L+1 (4%), H→L (2%), H→L+3 (4%) |
| | 590.176 | 2.101 | 0.111 | H→L (10%), H→L+2 (75%), H-3→L+1 (2%), H-2→L+1 (2%), H→L+4 (2%) |
| | 555.659 | 2.231 | 0.070 | H→L+3 (85%), H-2→L+2 (2%), H→L+1 (4%) |
| | 542.316 | 2.286 | 0.625 | H-1→L (59%), H-2→L (5%), H-2→L+1 (3%), H-1→L+2 (9%), H-1→L+4 (7%), H→L (4%) |
| | 533.747 | 2.323 | 0.062 | H-2→L (53%), H-3→L (2%), H-2→L+1 (4%), H-2→L+2 (6%), H-2→L+4 (7%), H-1→L (5%), H-1→L+1 (4%), H→L+1 (3%), H→L+3 (7%) |
| **A1D5** | 641.707 | 1.932 | 1.725 | H→L (83%), H-1→L (2%), H→L+2 (8%), H→L+4 (2%) |
| | 578.419 | 2.144 | 0.032 | H→L+1 (78%), H-2→L (5%), H-1→L+1 (6%), H→L+3 (2%) |
| | 566.837 | 2.187 | 0.094 | H→L+2 (74%), H-3→L+1 (4%), H-2→L+1 (4%), H-1→L (4%), H-1→L+2 (3%), H→L (5%), H→L+4 (2%) |
| | 534.253 | 2.321 | 0.610 | H-1→L (68%), H-1→L+2 (11%), H-1→L+4 (6%), H→L (4%), H→L+2 (2%) |
| | 530.504 | 2.337 | 0.092 | H-2→L (40%), H-2→L+2 (11%), H→L+3 (32%), H-2→L+4 (4%), H-1→L+3 (2%), H→L+1 (6%) |
| | 520.854 | 2.380 | 0.000 | H-2→L (27%), H→L+3 (58%), H-2→L+4 (4%), H-1→L+1 (4%) |

**Table S10:** Wave length, excitation energy and oscillator strength of **A1R1** and **A1D1-A1D5** in gas phase.

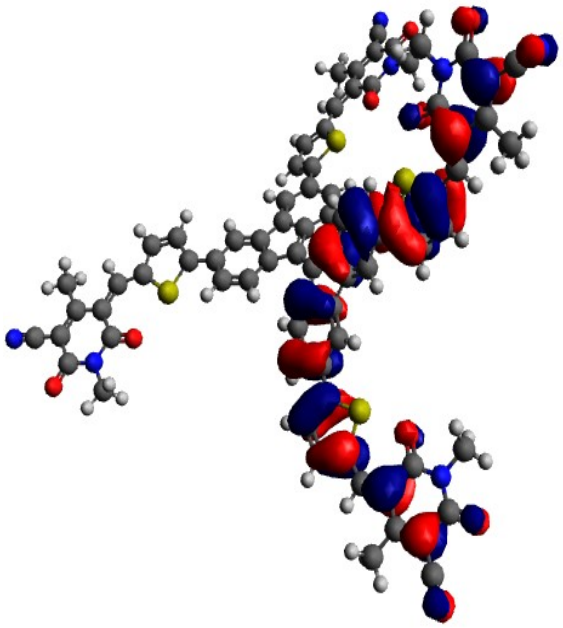
| **Compounds** | $\lambda$ (***nm***) | ***E*(*eV*)** | $f_{os}$ | **MO contributions** |
|---|---|---|---|---|
| **A1R** | 671.164 | 1.847 | 1.656 | H→L (97%), |
| | 580.478 | 2.136 | 0.374 | H-1→L (90%), H-5→L (5%) |
| | 569.153 | 2.178 | 0.562 | H-2→L (90%), H-6→L (6%) |
| | 508.445 | 2.439 | 0.836 | H→L+1 (92%), H→L+2 (4%) |
| | 506.203 | 2.449 | 0.467 | H→L+2 (91%), H→L+1 (3%) |
| | 491.591 | 2.522 | 0.041 | H-3→L (58%), H→L+3 (38%), |
| **A1D1** | 618.468 | 2.005 | 1.448 | H→L (89%), H→L+2 (4%) |
| | 568.474 | 2.181 | 0.020 | H→L+1 (85%), H-3→L+2 (2%), H-2→L (2%), H-1→L+1 (4%) |
| | 552.588 | 2.244 | 0.152 | H→L+2 (81%), H-3→L+1 (3%), H-2→L+1 (2%), H-1→L (3%) |

| | | | | |
|---|---|---|---|---|
| | 529.056 | 2.344 | 0.517 | H-1→L (68%), H-1→L+2 (11%), H-2→L (2%), H-1→L+4 (5%), H→L (3%), H→L+2 (2%) |
| | 521.556 | 2.377 | 0.085 | H-2→L (67%), H-2→L+2 (11%), H-2→L+4 (6%), H-1→L (2%), H→L+1 (3%) |
| | 507.487 | 2.443 | 0.019 | H→L+3 (81%), H-2→L+2 (3%), H-1→L+1 (6%) |
| **A1D2** | 649.676 | 1.908 | 1.243 | H→L (92%), H→L+4 (3%) |
| | 604.359 | 2.052 | 0.009 | H→L+1 (51%), H→L+2 (29%), H→L+3 (11%), H-2→L+1 (3%) |
| | 599.798 | 2.067 | 0.044 | H→L+1 (34%), H→L+2 (57%), |
| | 578.527 | 2.143 | 0.025 | H→L+3 (86%), H→L+1 (5%), H→L+2 (6%) |
| | 542.790 | 2.284 | 0.660 | H-2→L (37%), H-1→L (39%), H-2→L+4 (4%), H-1→L+3 (3%), H-1→L+4 (5%) |
| | 535.823 | 2.314 | 0.124 | H-2→L (36%), H-1→L (36%), H-2→L+1 (3%), H-2→L+3 (3%), H-2→L+4 (5%), H-1→L+4 (6%) |
| **A1D3** | 616.316 | 2.012 | 1.473 | H→L (90%), H→L+2 (3%) |
| | 563.488 | 2.200 | 0.026 | H→L+1 (83%), H-3→L+2 (2%), H-2→L (3%), H-1→L+1 (4%) |
| | 548.336 | 2.261 | 0.132 | H→L+2 (80%), H-3→L+1 (3%), H-2→L+1 (3%), H-1→L (4%) |
| | 527.525 | 2.350 | 0.492 | H-1→L (71%), H-1→L+2 (9%), H-1→L+4 (5%), H→L (3%), H→L+2 (3%) |
| | 520.264 | 2.383 | 0.078 | H-2→L (71%), H-2→L+2 (9%), H-2→L+4 (6%), H→L+1 (3%) |
| | 507.093 | 2.445 | 0.021 | H→L+3 (86%), H-2→L+2 (2%), H-1→L+1 (5%) |
| **A1D4** | 644.141 | 1.925 | 1.217 | H→L (73%), H→L+1 (15%), H→L+2 (6%) |
| | 607.468 | 2.041 | 0.035 | H→L (13%), H→L+1 (75%), H→L+3 (3%) |
| | 594.962 | 2.084 | 0.121 | H→L+2 (85%), H-2→L+2 (3%), H→L (6%) |
| | 562.593 | 2.204 | 0.035 | H→L+3 (94%), H→L+1 (2%) |
| | 540.920 | 2.292 | 0.549 | H-2→L (22%), H-1→L (43%), H-2→L+1 (5%), H-2→L+4 (2%), H-1→L+2 (7%), H-1→L+4 (5%), H→L (3%) |
| | 532.670 | 2.328 | 0.155 | H-2→L (27%), H-2→L+1 (23%), H-1→L (21%), H-2→L+3 (3%), H-2→L+4 (5%), H-1→L+1 (3%), H-1→L+2 (3%), H-1→L+4 (4%) |
| **A1D5** | 623.412 | 1.989 | 1.420 | H→L (89%), H→L+2 (4%) |
| | 574.986 | 2.156 | 0.017 | H→L+1 (85%), H-1→L+1 (3%) |
| | 563.565 | 2.200 | 0.119 | H→L+2 (83%), H-3→L+1 (3%), H→L (2%) |
| | 530.913 | 2.335 | 0.539 | H-1→L (65%), H-2→L (6%), H-1→L+2 (7%), H-1→L+4 (6%), H→L (2%), H→L+3 (2%) |
| | 527.390 | 2.351 | 0.080 | H-2→L (10%), H→L+3 (79%), H-2→L+2 (3%) |
| | 523.206 | 2.370 | 0.037 | H-2→L (55%), H→L+3 (13%), H-2→L+2 (4%), H-2→L+4 (6%), H-1→L (8%) |

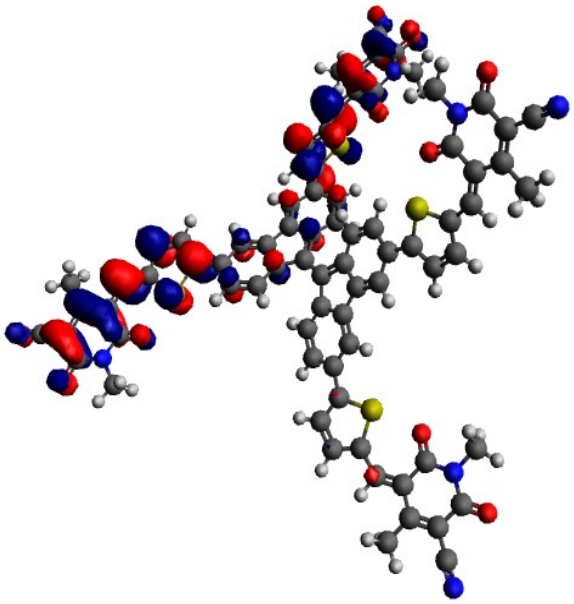
**Table S11:** GRP values of the investigated compounds (**A1R** and **A1D1**-**A1D5**).

| Compounds | *IP* | *EA* | *X* | *η* | *μ* | *ω* | *σ* | $\Delta N_{max}$ |
|---|---|---|---|---|---|---|---|---|
| **A1R** | 6.302 | 3.557 | 4.929 | 1.372 | -4.929 | 8.852 | 0.364 | 3.592 |
| **A1D1** | 5.623 | 3.136 | 4.379 | 1.243 | -4.379 | 7.712 | 0.402 | 3.522 |
| **A1D2** | 5.684 | 3.330 | 4.507 | 1.177 | -4.507 | 8.629 | 0.424 | 3.382 |
| **A1D3** | 5.616 | 3.130 | 4.373 | 1.243 | -4.373 | 7.692 | 0.402 | 3.518 |
| **A1D4** | 5.672 | 3.263 | 4.467 | 1.204 | -4.467 | 8.284 | 0.415 | 3.710 |
| **A1D5** | 6.149 | 3.158 | 4.653 | 1.499 | -4.653 | 7.240 | 0.334 | 3.103 |

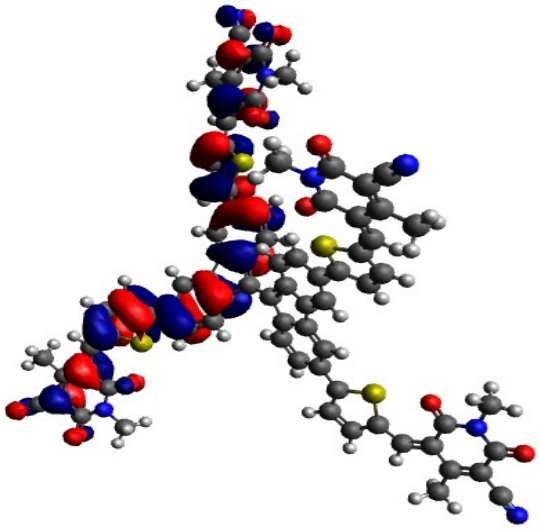
All properties are in *eV,* while *σ* is in $eV^{-1}$



**HOMO -1**



**LUMO +1**



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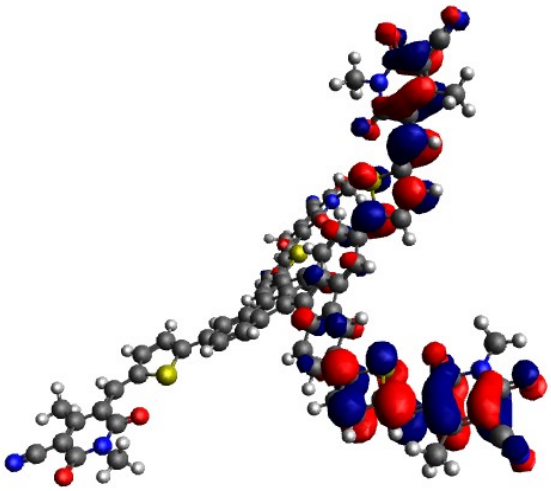
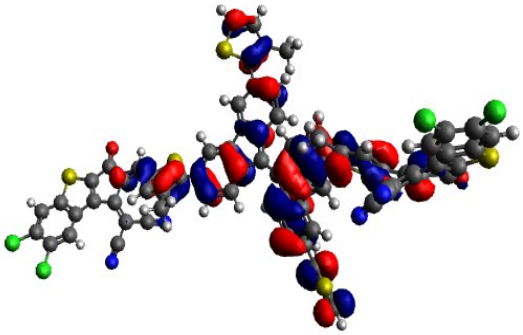


**LUMO +2**

**A1R**



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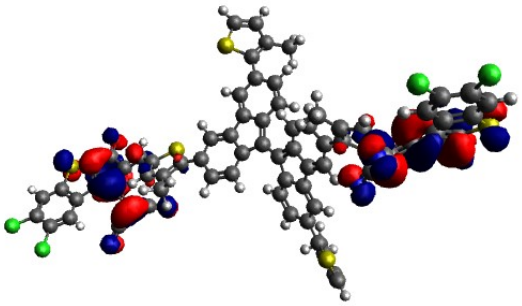

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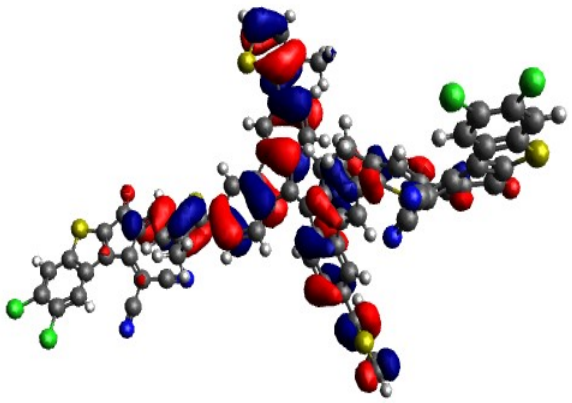

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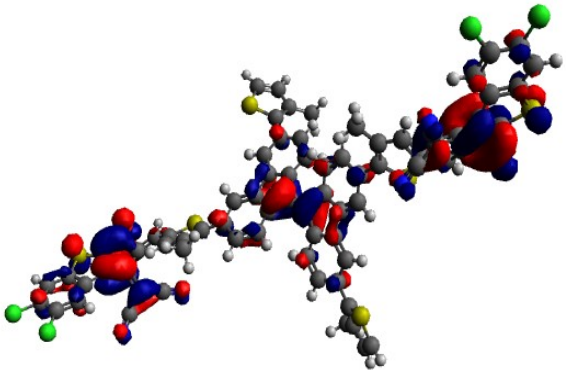
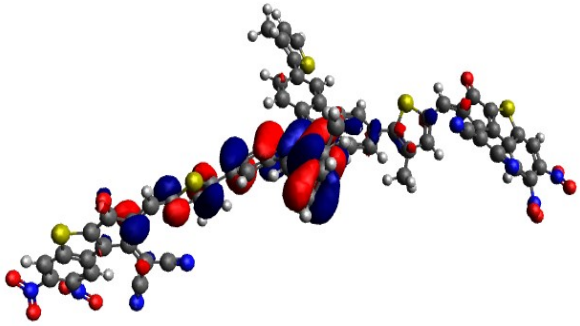
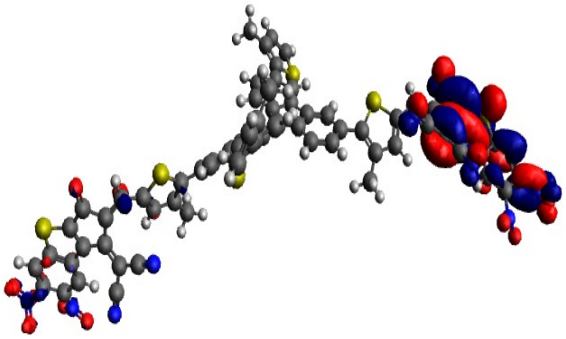


LUMO +2

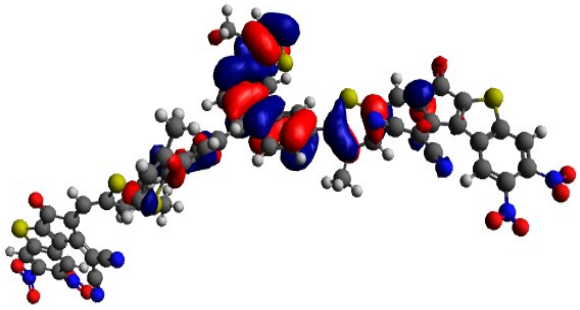
**A1D1**



HOMO -1



LUMO +1



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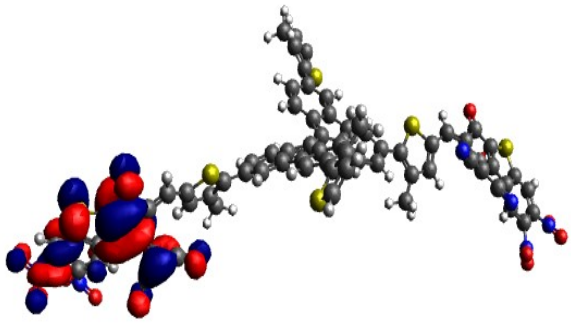
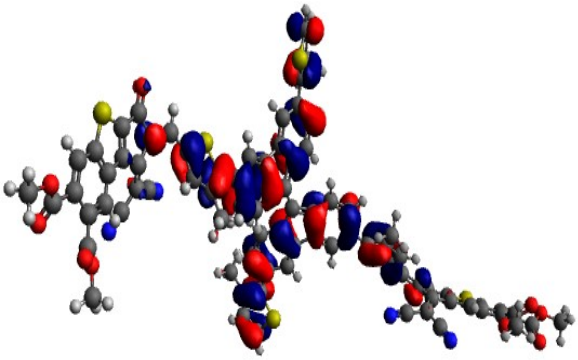
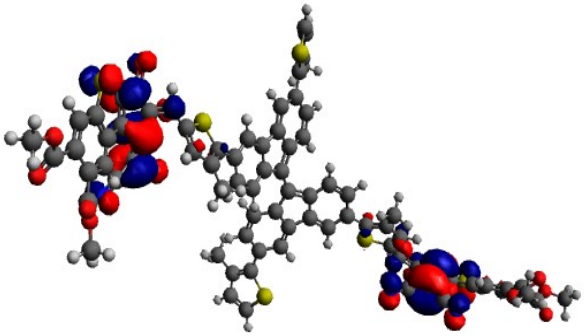


LUMO +2

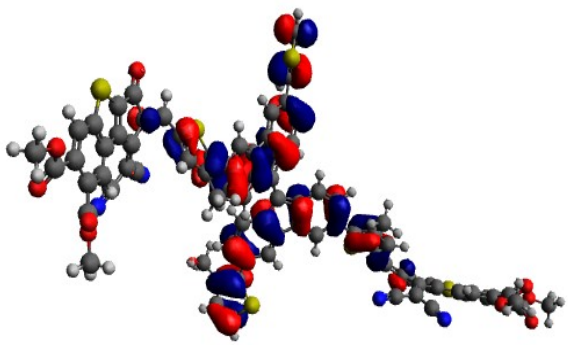
**A1D2**



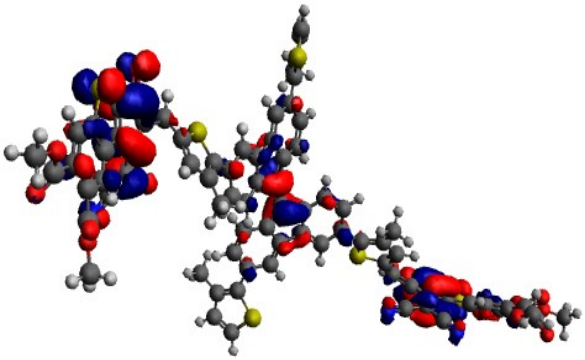
HOMO -1



LUMO +1

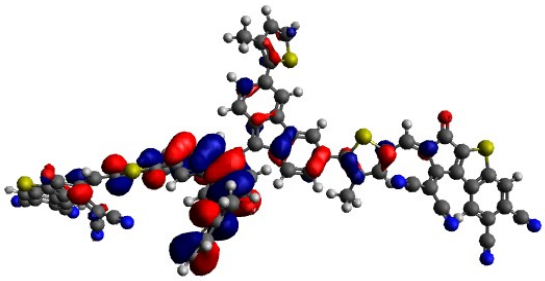


HOMO -2

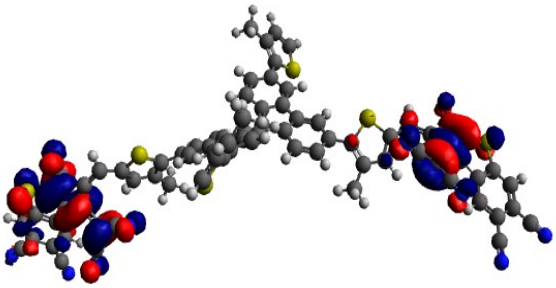


LUMO +2

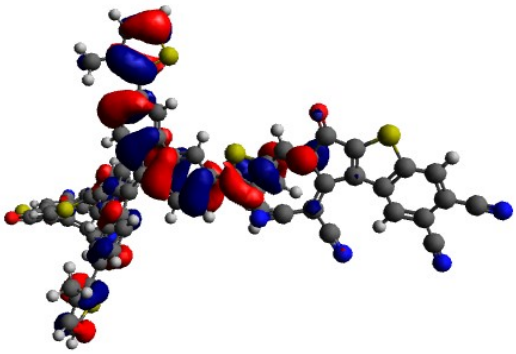
**A1D3**



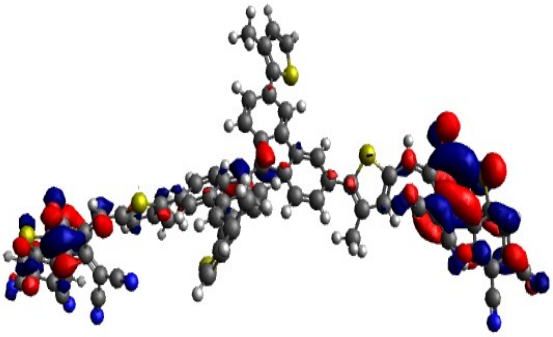
HOMO -1



LUMO +1

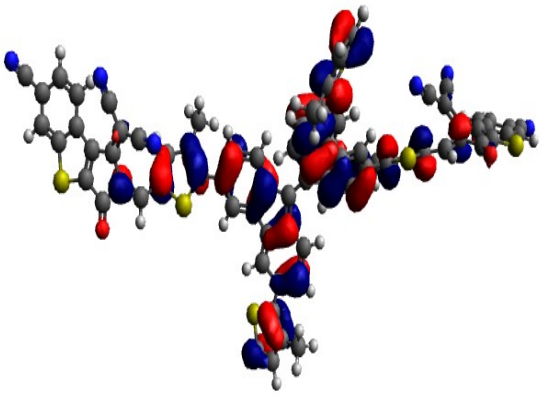


HOMO -2

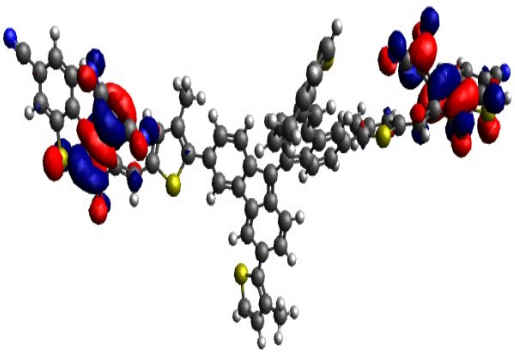


LUMO +2

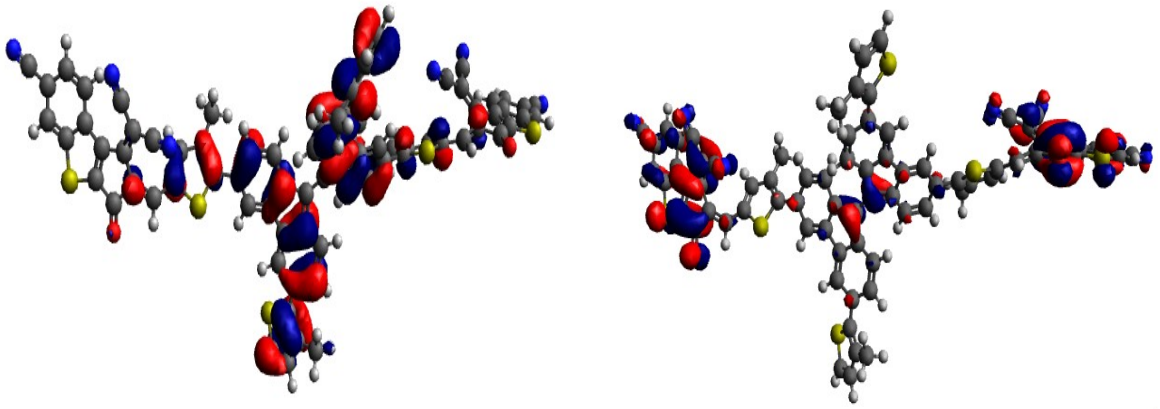
**A1D4**



HOMO -1



LUMO +1



**HOMO -2** **LUMO +2**

**A1D5**

**Figure S1:** HOMO-1/LUMO+1 and HOMO-2/LUMO+2 of the studied compounds (**A1R** and **A1D1-A1D5**).

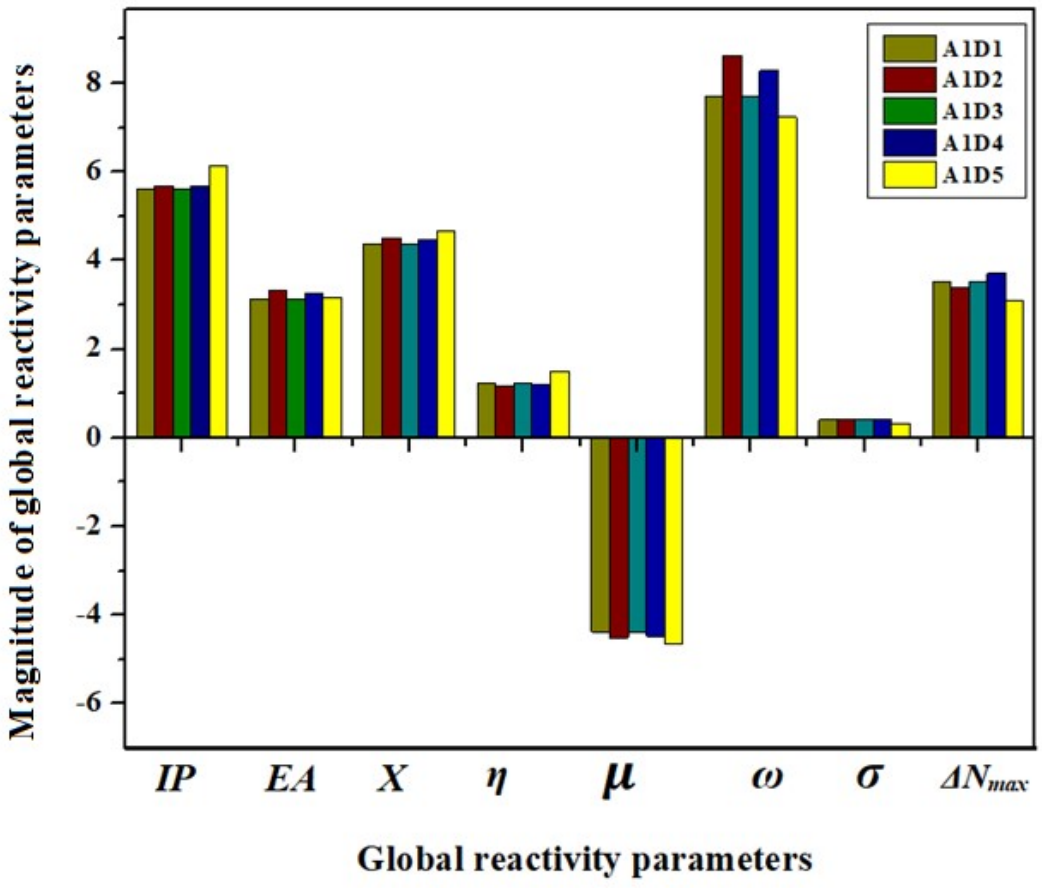
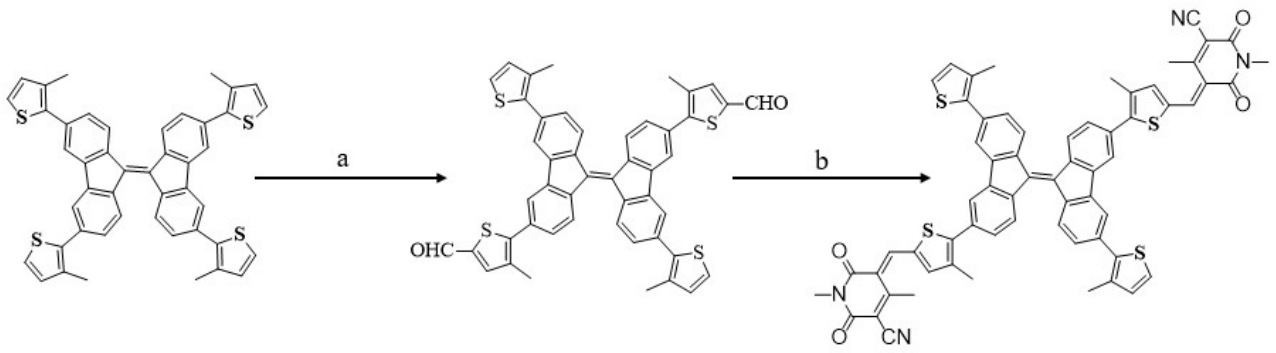



**Figure S2:** Bar graph representation of GRP values of the studied compounds.




**Scheme 1**: The synthetic pathway of **A1R** chromophore. a) -78$^0$C, DMF, n-BuLi, THF b) 100$^0$C, IC, n-BuOH.[1]

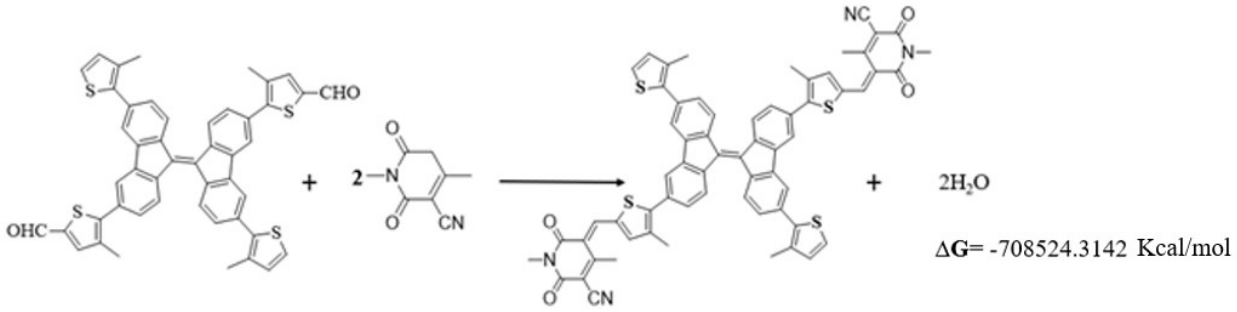



**Table S12**: Theoretically calculated values of Gibbs free energy for entitled chromophores in Kcal/mol at T=298.15 K and pressure 1 atm.

| Compounds | $\sum(\varepsilon_\circ + G_{corr})_{products}$ | $\sum(\varepsilon_\circ + G_{corr})_{reactants}$ | $\Delta_r G^\circ(298K)$ |
|---|---|---|---|
| **A1R** | -3580909.22 | -2872384.90 | -708524.31 |
| **A1D1** | -4762859.11 | -4716408.58 | -46450.54 |
| **A1D2** | -4122369.90 | -3093105.50 | -1029264.40 |
| **A1D3** | -4180906.02 | -4134457.91 | -46448.11 |
| **A1D4** | -3840701.11 | -3794249.24 | -46451.87 |
| **A1D5** | -3725004.80 | -2894423.90 | -830580.90 |

All the values are calculated by using Eq S1[2].

$$\Delta_r G^\circ(298K) = \sum(\varepsilon_\circ + G_{corr})_{products} - \sum(\varepsilon_\circ + G_{corr})_{reactants} \qquad \text{Eq S1}$$

## References


1. Wei, T. Zhang, Y. Zhao, Y. Zhou, M. Hailin and T. Yu, *New Journal of Chemistry*, 2021, **45**, 7637–7646.
2. Ochterski, J. W. Thermochemistry in gaussian. *Gaussian Inc*, 2000. ***1***,1.