Supplementary Information

Structural Parameters Modulated Nonlinear Optical Amplitude of Acceptor-π-D-π-Donor Configurated Pyrene Derivatives: A DFT Approach

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**Table S1: Cartesian coordinates of MCPTR**

| Atom | X-axis   | Y-axis   | Z-axis   |
|------|----------|----------|----------|
| C    | -3.45168 | -2.65703 | 0.260534 |
| C    | -4.81187 | -2.82556 | 0.43042  |
| C    | -5.68739 | -1.74856 | 0.266557 |
| C    | -5.1573  | -0.47855 | -0.09227 |
| C    | -3.75326 | -0.30401 | -0.27515 |
| C    | -2.89681 | -1.41532 | -0.08143 |
| C    | -7.09901 | -1.89431 | 0.450339 |
| C    | -6.04691 | 0.618344 | -0.2755  |
| C    | -7.44625 | 0.445994 | -0.0878  |
| C    | -7.94095 | -0.84506 | 0.282313 |
| C    | -8.29955 | 1.538612 | -0.27116 |
| H    | -9.36943 | 1.399943 | -0.12418 |
| C    | -7.79773 | 2.781622 | -0.63483 |
| C    | -6.43402 | 2.958303 | -0.82525 |
| C    | -5.54489 | 1.892014 | -0.65224 |
| C    | -4.13833 | 2.030431 | -0.86247 |
| C    | -3.2877  | 0.987155 | -0.69061 |
| H    | -2.22946 | 1.129849 | -0.88753 |
| H    | -3.75591 | 2.999167 | -1.17945 |
| H    | -7.48048 | -2.87491 | 0.729808 |
| H    | -2.78006 | -3.49608 | 0.427724 |
| H    | -5.21248 | -3.79813 | 0.71036  |
| H    | -9.01382 | -0.96466 | 0.424058 |
| H    | -8.47684 | 3.61926  | -0.77273 |
| H    | -6.03927 | 3.930773 | -1.11449 |
| C    | 2.359539 | -0.5233  | 0.174609 |
| H    | 3.115744 | -1.18968 | -0.23987 |
| C    | 2.837706 | 0.576879 | 0.816227 |
| C    | 1.9782   | 1.548097 | 1.407477 |
| N    | 1.249094 | 2.323463 | 1.878541 |
| C    | 4.287437 | 0.849676 | 0.946233 |
| O    | 4.742973 | 1.819275 | 1.504935 |
| O    | 5.036862 | -0.10756 | 0.372793 |
| C    | 6.454079 | 0.091934 | 0.456246 |
| C    | 7.11632  | -1.07094 | -0.24274 |
| H    | 6.748238 | 0.15287  | 1.513667 |
| H    | 6.701608 | 1.057538 | -0.00236 |
| C    | 8.632847 | -1.05536 | -0.10274 |
| H    | 6.709798 | -2.00164 | 0.175297 |
| H    | 6.835899 | -1.05657 | -1.30627 |
| H    | 9.040017 | -1.96154 | -0.57421 |
| H    | 8.90519  | -1.12483 | 0.962631 |
| Atom | X-axis | Y-axis | Z-axis |
|------|--------|--------|--------|
| C    | 9.307256 | 0.165079 | -0.7142 |
| C    | 10.82469 | 0.061221 | -0.71436 |
| H    | 9.012256 | 1.076374 | -0.17011 |
| H    | 8.948684 | 0.303909 | -1.74802 |
| C    | 11.49627 | 1.290498 | -1.30104 |
| H    | 11.17512 | -0.10236 | 0.316091 |
| H    | 11.12368 | -0.83584 | -1.27769 |
| H    | 12.58744 | 1.200117 | -1.30267 |
| H    | 11.17491 | 1.4581 | -2.33663 |
| H    | 11.23806 | 2.190856 | -0.72989 |
| C    | 1.021254 | -0.95902 | -0.04562 |
| C    | 0.702328 | -2.10779 | -0.74878 |
| S    | -0.43429 | -0.15903 | 0.507128 |
| C    | -0.67475 | -2.34287 | -0.84818 |
| H    | 1.467686 | -2.74572 | -1.18261 |
| C    | -1.43978 | -1.37463 | -0.22813 |
| H    | -1.11881 | -3.18176 | -1.37527 |

Table S2: Cartesian coordinates of MCPTD1
|   |   |   |   |
|---|---|---|---|
| C | -12.3369 | -0.36047 | 0.082756 |
| H | -13.1552 | -0.86664 | 0.594759 |
| C | -12.6763 | 0.779647 | -0.5777 |
| C | -11.7217 | 1.560228 | -1.29283 |
| N | -10.9183 | 2.176556 | -1.86686 |
| C | -14.0624 | 1.299973 | -0.59982 |
| O | -14.3915 | 2.313888 | -1.16866 |
| O | -14.9115 | 0.514259 | 0.084911 |
| C | -16.2744 | 0.959393 | 0.102405 |
| C | -17.0664 | -0.03098 | 0.921356 |
| H | -16.6467 | 1.022683 | -0.93005 |
| H | -16.3093 | 1.974002 | 0.518387 |
| C | -18.5621 | 0.257088 | 0.901896 |
| H | -18.8734 | -1.03809 | 0.528226 |
| H | -18.6932 | -0.02077 | 1.955883 |
| H | -19.0811 | -0.53396 | 1.462343 |
| H | -18.9367 | 0.185582 | -0.13192 |
| C | -18.9501 | 1.610018 | 1.482612 |
| C | -20.4557 | 1.787688 | 1.606756 |
| H | -18.5465 | 2.423564 | 0.859227 |
| H | -18.4831 | 1.73293 | 2.474437 |
| C | -20.8417 | 3.149087 | 2.157954 |
| H | -20.9187 | 1.637081 | 0.61958 |
| H | -20.8604 | 0.99256 | 2.25111 |
| H | -21.9269 | 3.261501 | 2.250639 |
| H | -20.4046 | 3.309544 | 3.151542 |
| H | -20.4783 | 3.954731 | 1.508104 |
| C | -11.0763 | -1.01079 | 0.216773 |
| C | -10.8874 | -2.16715 | 0.95381 |
| S | -9.56457 | -0.48766 | -0.49286 |
| C | -9.56262 | -2.6234 | 0.957313 |
| H | -11.705 | -2.65089 | 1.481704 |
| C | -8.70776 | -1.82043 | 0.228512 |
| H | -9.21739 | -3.502 | 1.493811 |
| C | -0.1759 | -0.18422 | -1.09744 |
| C | 0.263406 | -0.84944 | -2.21567 |
| S | 1.186711 | 0.426375 | -0.19022 |
| C | 1.670315 | -0.86304 | -2.35363 |
| H | -0.42012 | -1.27228 | -2.94668 |
| C | 2.331545 | -0.20897 | -1.34286 |
| H | 2.186718 | -1.31017 | -3.19833 |
| C | 3.767829 | -0.03893 | -1.15769 |
| C | 4.30034 | 1.012271 | -0.39993 |
| C | 4.671165 | -0.93699 | -1.74353 |
|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 5.665877  | 1.158899  | -0.22647  |
| H | 3.630496  | 1.735933  | 0.062184  |
| C | 6.038044  | -0.78314  | -1.597    |
| H | 4.291519  | -1.77832  | -2.31949  |
| C | 6.559994  | 0.266066  | -0.82927  |
| H | 6.052724  | 1.976877  | 0.376164  |
| H | 6.718762  | -1.48868  | -2.0675   |
| N | 7.950819  | 0.410009  | -0.66443  |
| C | 8.771829  | -0.74017  | -0.54391  |
| C | 9.976048  | -0.81451  | -1.25479  |
| C | 8.383248  | -1.79624  | 0.285464  |
| C | 10.0046   | -1.93022  | -1.14095  |
| H | 10.25583  | 0.018887  | -1.89521  |
| H | 7.448308  | -1.7309   | 0.839694  |
| C | 10.41129  | -2.98434  | -0.33066  |
| H | 11.73474  | -1.9725   | -1.70051  |
| C | 8.541916  | 1.695218  | -0.58706  |
| C | 9.546348  | 1.945314  | 0.352799  |
| C | 8.132952  | 2.712208  | -1.46029  |
| H | 9.858623  | 1.152953  | 1.030941  |
| C | 8.704783  | 3.97946   | -1.39224  |
| H | 7.358516  | 2.496717  | -2.19249  |
| C | 9.706319  | 4.227114  | -0.4678   |
| H | 8.371989  | 4.760329  | -2.07582  |
| C | 10.12748  | 3.20509   | 0.395426  |
| C | 11.18278  | 3.736628  | 1.256382  |
| C | 10.47411  | 5.08248   | -0.21049  |
| C | 9.201251  | -2.91412  | 0.375581  |
| C | 9.046263  | -4.14779  | 1.144777  |
| C | 11.12139  | -4.2968   | -0.06605  |
| C | 10.15999  | -4.96422  | 0.898427  |
| C | 10.26803  | -6.20393  | 1.506958  |
| C | 8.033259  | -4.56726  | 2.00036   |
| C | 9.253603  | -6.62551  | 2.366367  |
| H | 11.13132  | -6.84187  | 1.318253  |
| C | 8.146856  | -5.81335  | 2.609546  |
| H | 7.16807   | -3.93468  | 2.19151   |
| H | 9.325706  | -7.59616  | 2.851598  |
| H | 7.365083  | -6.15807  | 3.282389  |
| C | 11.3987   | 5.079516  | 0.912358  |
| C | 12.35696  | 5.826805  | 1.577374  |
| C | 11.92382  | 3.134361  | 2.267171  |
| C | 13.10102  | 5.22406   | 2.591339  |
| H | 12.52933  | 6.870344  | 1.314183  |
**Table S3: Cartesian coordinates of MCPTD2**

| Atom | X-axis  | Y-axis  | Z-axis  |
|------|---------|---------|---------|
| C    | 7.168105| -1.50244| 3.507513|
| C    | 5.857444| -1.49365| 3.938431|
| C    | 4.805422| -1.49386| 3.016703|
| C    | 5.099273| -1.53202| 1.627047|
| C    | 6.455481| -1.54134| 1.180972|
| C    | 7.495934| -1.50643| 2.14344 |
| C    | 3.442841| -1.42975| 3.435384|
| C    | 4.026529| -1.55892| 0.686208|
| C    | 2.671182| -1.54813| 1.131418|
| C    | 2.424999| -1.44678| 2.538427|
| C    | 1.626449| -1.60425| 0.17528 |
| C    | 1.952598| -1.60989| -1.18812|
| C    | 3.263623| -1.60323| -1.62077|
| C    | 4.318152| -1.59546| -0.70279|
| C    | 5.679955| -1.64538| -1.12215|
| C    | 6.699794| -1.62932| -0.22742|
| H    | 7.722419| -1.69781| -0.5846 |
| H    | 5.88795 | -1.71043| -2.18877|
| H    | 3.236694| -1.34875| 4.501317 |
| H    | 7.974286| -1.45912| 4.23631 |
| H    | 5.629735| -1.46395| 5.002301 |
|   |   |   |   |
|---|---|---|---|
| H | 1.39829 | -1.36281 | 2.881994 |
| H | 1.147715 | -1.66168 | -1.91842 |
| H | 3.489504 | -1.62868 | -2.68529 |
| C | 12.47243 | -0.49292 | 0.47965 |
| H | 13.28435 | -1.02135 | 0.975694 |
| C | 11.2284 | -0.8971 | 1.027576 |
| C | 11.19373 | -1.85093 | 2.044124 |
| S | 9.596999 | -0.38609 | 0.63239 |
| C | 9.911651 | -2.16333 | 2.490462 |
| H | 12.1067 | -2.30055 | 2.427112 |
| C | 8.922098 | -1.4629 | 1.818843 |
| H | 9.690799 | -2.89516 | 3.261404 |
| C | 0.2156 | -1.67313 | 0.556744 |
| C | -0.40478 | -2.44303 | 1.510106 |
| S | -0.97272 | -0.74515 | -0.32671 |
| C | -1.81044 | -2.29295 | 1.537712 |
| H | 0.142402 | -3.12841 | 2.151236 |
| H | -2.4547 | -2.81675 | 2.238024 |
| N | -7.69883 | -0.01609 | -0.51109 |
| C | -8.12743 | 1.335279 | -0.50082 |
| C | -8.92641 | 1.820656 | -1.54451 |
| C | -7.76155 | 2.181402 | 0.550487 |
| C | -9.37078 | 3.139273 | -1.5444 |
| H | -9.19376 | 1.14080 | -2.35587 |
| H | -7.14816 | 1.797324 | 1.363923 |
| C | -9.00094 | 3.982898 | -0.51 |
| H | -9.99347 | 3.500304 | -2.36267 |
| C | -8.61928 | -1.033 | -0.86924 |
| C | -9.91659 | -1.01588 | -0.348 |
| C | -8.23495 | -2.04801 | -1.75516 |
| H | -10.2115 | -0.22467 | 0.339283 |
| C | -9.12496 | -3.05751 | -2.10948 |
| C | -10.4119 | -3.04063 | -1.59773 |
| H | -8.80789 | -3.84183 | -2.7965 |
| C | -10.804 | -2.01447 | -0.72524 |
| C | -12.1972 | -2.24349 | -0.3486 |
| C | -11.5469 | -4.0148 | -1.8399 |
| C | -8.19161 | 3.501164 | 0.530063 |
| C | -7.96141 | 4.592183 | 1.476253 |
| C | -9.34951 | 5.441992 | -0.29734 |
| C | -8.63068 | 5.732009 | 1.005577 |
| C | -8.57486 | 6.920059 | 1.715222 |
| C | -7.2318 | 4.635572 | 2.659371 |
| C | -7.84402 | 6.964827 | 2.902107 |
|      |       |       |       |
|------|-------|-------|-------|
|      |       |       |       |
| H    | -9.0926 | 7.808167 | 1.353382 |
| C    | -7.17861 | 5.831778 | 3.368502 |
| H    | -6.70992 | 3.752368 | 3.023928 |
| H    | -7.7918 | 7.890973 | 3.469819 |
| H    | -6.61227 | 5.884256 | 4.295428 |
| C    | -12.6446 | -3.40733 | -0.9879 |
| C    | -13.941 | -3.85754 | -0.80029 |
| C    | -13.0457 | -1.5228 | 0.488757 |
| C    | -14.7926 | -3.13635 | 0.036321 |
| H    | -14.2925 | -4.76142 | -1.29761 |
| C    | -14.3472 | -1.97951 | 0.67414 |
| H    | -12.7003 | -0.61834 | 0.986831 |
| H    | -15.8129 | -3.47849 | 0.193347 |
| H    | -15.0244 | -1.42846 | 1.322583 |
| C    | -8.81244 | 6.314773 | -1.43416 |
| H    | -7.72983 | 6.188824 | -1.54725 |
| H    | -9.29099 | 6.049066 | -2.38535 |
| H    | -9.01645 | 7.37525 | -1.23911 |
| C    | -10.8607 | 5.637012 | -0.1521 |
| H    | -11.0977 | 6.686108 | 0.06624 |
| H    | -11.3779 | 5.360484 | -1.07958 |
| H    | -11.2592 | 5.019075 | 0.660389 |
| C    | -11.183 | -5.42096 | -1.35775 |
| H    | -10.3399 | -5.82134 | -1.93496 |
| H    | -10.9003 | -5.41099 | -0.29911 |
| H    | -12.0311 | -6.10627 | -1.48065 |
| C    | -11.9461 | -4.05006 | -3.31684 |
| H    | -11.1205 | -4.42928 | -3.93246 |
| H    | -12.8104 | -4.70874 | -3.46953 |
| H    | -12.2099 | -3.0488 | -3.67551 |
| C    | 12.75074 | 2.04257 | -2.18992 |
| C    | 14.1021 | 1.731073 | -1.98812 |
| C    | 15.07032 | 2.390689 | -2.74472 |
| C    | 14.65045 | 3.337617 | -3.67636 |
| C    | 13.30015 | 3.634998 | -3.8657 |
| C    | 12.32938 | 2.980938 | -3.11398 |
| C    | 11.9162 | 1.232717 | -1.28385 |
| C    | 12.84066 | 0.394163 | -0.49774 |
| C    | 14.20108 | 0.693843 | -0.93858 |
| H    | 16.12962 | 2.19006 | -2.6287 |
| H    | 15.39911 | 3.856844 | -4.26927 |
| H    | 13.01141 | 4.379435 | -4.6027 |
| H    | 11.26762 | 3.184373 | -3.23013 |
| O    | 10.69907 | 1.268072 | -1.21148 |
| Atom | X-axis  | Y-axis  | Z-axis  |
|------|--------|--------|--------|
| C    | 15.38174 | 0.139257 | -0.498 |
| C    | 16.65858 | 0.515859 | -1.01006 |
| N    | 17.71608 | 0.800093 | -1.40569 |
| C    | 15.46124 | -0.86896 | 0.507683 |
| N    | 15.54641 | -1.69267 | 1.326771 |
| H    | -7.22498 | -2.03564 | -2.15848 |
| C    | -3.67265 | -1.02629 | 0.332689 |
| C    | -3.99946 | 0.165614 | -0.32683 |
| C    | -4.72992 | -1.86386 | 0.715686 |
| C    | -5.31291 | 0.500001 | -0.60889 |
| H    | -3.20809 | 0.849624 | -0.62968 |
| C    | -6.04664 | -1.52625 | 0.459717 |
| H    | -4.51396 | -2.8065 | 1.214221 |
| C    | -6.36119 | -0.34202 | -0.21952 |
| H    | -5.53748 | 1.423918 | -1.13615 |
| H    | -6.84958 | -2.19049 | 0.770465 |
| C    | -2.29091 | -1.40653 | 0.604602 |

| Atom | X-axis  | Y-axis  | Z-axis  |
|------|--------|--------|--------|
| C    | 6.652865 | -4.20884 | -0.06605 |
| C    | 5.348465 | -4.54589 | 0.229635 |
| C    | 4.328968 | -3.59265 | 0.138735 |
| C    | 4.646636 | -2.27462 | -0.28789 |
| C    | 5.993729 | -1.93155 | -0.61545 |
| C    | 7.007455 | -2.91316 | -0.47273 |
| C    | 2.972814 | -3.91603 | 0.441675 |
| C    | 3.605674 | -1.30448 | -0.39053 |
| C    | 2.265998 | -1.63703 | 0.0297 |
| C    | 1.988301 | -2.98594 | 0.361199 |
| C    | 1.258953 | -0.64338 | -0.10781 |
| C    | 1.592488 | 0.625364 | -0.60204 |
| C    | 2.883279 | 0.941105 | -0.97705 |
| C    | 3.909906 | -0.00148 | -0.86577 |
| C    | 5.252127 | 0.300514 | -1.23904 |
| C    | 6.245871 | -0.61615 | -1.12279 |
| H    | 7.249156 | -0.35389 | -1.44299 |
| H    | 5.465435 | 1.291735 | -1.63549 |
| H    | 2.740762 | -4.94058 | 0.727514 |
| H    | 7.439147 | -4.95006 | 0.057125 |
| H    | 5.103221 | -5.55496 | 0.555419 |
| H    | 0.959833 | -3.26459 | 0.570822 |
| H    | 0.815324 | 1.384945 | -0.65722 |
| H    | 3.117947 | 1.937694 | -1.34672 |
|   |   |   |   |
|---|---|---|---|
|   |   |   |   |
| C | 12.10335 | -1.31981 | -0.64083 |
| H | 12.82826 | -1.99186 | -1.09664 |
| C | 10.80753 | -1.88802 | -0.7061 |
| C | 10.62069 | -3.13407 | -1.30606 |
| S | 9.270202 | -1.2679 | -0.12842 |
| C | 9.300777 | -3.57565 | -1.30446 |
| H | 11.45343 | -3.68316 | -1.73873 |
| C | 8.43033 | -2.6738 | -0.70999 |
| H | 8.96486 | -4.51038 | -1.74262 |
| C | 9.300777 | -3.57565 | -1.30446 |
| C | -0.11824 | -1.47622 | 1.46616 |
| S | -1.44994 | -0.32285 | -0.65907 |
| C | -2.00332 | -1.45943 | 1.572119 |
| H | 0.066241 | -1.86037 | 2.239141 |
| H | -2.543 | -1.84249 | 2.433443 |
| N | -8.20985 | -0.1156 | -0.35756 |
| C | -8.71281 | 1.161406 | -0.72268 |
| C | -9.59496 | 1.271502 | -1.80373 |
| C | -8.34115 | 2.299259 | -0.00126 |
| C | -10.1117 | 2.509399 | -2.17492 |
| H | -9.8687 | 0.370396 | -2.34812 |
| H | -7.66223 | 2.203824 | 0.844745 |
| C | -9.73463 | 3.641302 | -1.47111 |
| H | -10.7969 | 2.580461 | -3.01927 |
| C | -9.12874 | -1.18651 | -0.21709 |
| C | -10.3271 | -0.97986 | 0.472043 |
| C | -8.85477 | -2.4368 | -0.78627 |
| H | -10.531 | -0.00417 | 0.910579 |
| C | -9.76034 | -3.48657 | -0.65987 |
| C | -10.9519 | -3.28256 | 0.01702 |
| H | -9.53368 | -4.45432 | -1.10693 |
| C | -11.2322 | -2.0268 | 0.575636 |
| C | -12.5382 | -2.09509 | 1.228718 |
| C | -12.0832 | -4.25764 | 0.274389 |
| C | -8.84894 | 3.532407 | -0.38839 |
| C | -8.64434 | 4.867027 | 0.173447 |
| C | -10.1517 | 5.081485 | -1.69122 |
| C | -9.39966 | 5.781407 | -0.57621 |
| C | -9.3902 | 7.128434 | -0.25392 |
| C | -7.87677 | 5.295524 | 1.250953 |
| C | -8.62235 | 7.559204 | 0.827587 |
| H | -9.97489 | 7.842423 | -0.83372 |
| C | -7.8731 | 6.649425 | 1.572555 |
| H | -7.29019 | 4.587194 | 1.833516 |
| Element | X   | Y     | Z     |
|---------|-----|-------|-------|
| H       | -8.60734 | 8.613555 | 1.093647 |
| H       | -7.28012 | 7.002025 | 2.413201 |
| C       | -13.0472 | -3.39161 | 1.062559 |
| C       | -14.2817 | -3.73242 | 1.59029  |
| C       | -13.2611 | -1.13182 | 1.923821 |
| C       | -15.0076 | -2.76777 | 2.288769 |
| H       | -14.6818 | -4.73819 | 1.462957 |
| C       | -14.5004 | -1.47941 | 2.452794 |
| H       | -12.8659 | -0.12562 | 2.053022 |
| H       | -15.978  | -3.02119 | 2.709421 |
| H       | -15.0798 | -0.73947 | 3.000044 |
| C       | -9.69995 | 5.5851  | -3.06418 |
| H       | -8.6175  | 5.467522 | -3.18764 |
| H       | -10.2001 | 5.026845 | -3.86572 |
| H       | -9.94618 | 6.647182 | -3.18827 |
| C       | -11.6643 | 5.253011 | -1.53759 |
| H       | -11.9476 | 6.308674 | -1.63497 |
| H       | -12.1981 | 4.688479 | -2.31261 |
| H       | -12.0025 | 4.895902 | -0.55841 |
| C       | -11.6087 | -5.45469 | 1.101585 |
| H       | -10.8607 | -6.03626 | 0.547794 |
| H       | -11.1581 | -5.12549 | 2.04471  |
| H       | -12.4478 | -6.12162 | 1.336753 |
| C       | -12.7125 | -4.73849 | -1.03528 |
| H       | -11.986  | -5.31033 | -1.6266  |
| H       | -13.5729 | -5.39   | -0.8366  |
| H       | -13.0562 | -3.89129 | -1.63935 |
| C       | 12.76814 | 1.954474 | 0.929866 |
| C       | 14.06103 | 1.592856 | 0.53419  |
| C       | 15.12611 | 2.450059 | 0.815879 |
| C       | 14.84363 | 3.630416 | 1.481366 |
| C       | 13.5438  | 3.974945 | 1.869013 |
| C       | 12.48251 | 3.133613 | 1.595303 |
| C       | 11.81561 | 0.900883 | 0.535207 |
| C       | 12.60564 | -0.1488  | -0.1321  |
| C       | 14.00161 | 0.280178 | -0.143   |
| H       | 16.1579  | 2.248446 | 0.54811  |
| H       | 11.46859 | 3.387913 | 1.891332 |
| O       | 10.61322 | 0.921945 | 0.737059 |
| C       | 15.09342 | -0.37029 | -0.67133 |
| C       | 16.4139  | 0.165344 | -0.61798 |
| N       | 17.5004  | 0.582579 | -0.58691 |
| C       | 15.02648 | -1.63602 | -1.32464 |
| N       | 14.99184 | -2.66942 | -1.86064 |
Table S5: Cartesian coordinates of MCPTD4

| Atom | X-axis  | Y-axis  | Z-axis  |
|------|---------|---------|---------|
| C    | 6.472233| -4.34735| -0.07316|
| C    | 5.16507 | -4.67695| 0.217671|
| C    | 4.150444| -3.71907| 0.118904|
| C    | 4.476057| -2.40476| -0.31304|
| C    | 5.825943| -2.06984| -0.63821|
| C    | 6.835277| -3.05505| -0.48411|
| C    | 2.792039| -4.03405| 0.420097|
| C    | 3.440392| -1.42958| -0.42152|
| C    | 2.098547| -1.75277| -0.05991|
| C    | 1.812737| -3.09869| 0.335004|
| C    | 1.097658| -0.75295| -0.14056|
| C    | 1.439031| 0.511786| -0.63997|
| C    | 2.731398| 0.817869| -1.017|
| C    | 3.752288| -0.13045| -0.90186|
| C    | 5.096008| 0.16214| -1.27611|
| C    | 6.084861| -0.75907| -1.15368|
| H    | 7.089148| -0.50312| -1.47534|
| H    | 5.315165| 1.149935| -1.67776|
| H    | 2.553929| -5.05627| 0.709209|
| H    | 7.25408 | -5.09168| 0.059078|
| H    | 4.913773| -5.68323| 0.547422|
| H    | 0.782393| -3.37085| 0.544125|
| H    | 0.667075| 1.276468| -0.69695|
| H    | 2.972225| 1.811599| -1.39031|
| C    | 11.92916| -1.45795| -0.63365|
| H    | 12.65865| -2.13893| -1.06814|
| C    | 10.63687| -2.03169| -0.69311|
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 10.45822| -3.29161| -1.26875|
| S       | 9.091802| -1.40304| -0.14562|
| C       | 9.139762| -3.73465| -1.2736 |
| H       | 11.29661| -3.82099| -0.70826|
| C       | 8.260494| -4.67841| -1.69717|
| C       | -0.28002| -0.98854| 0.290231|
| C       | -0.75667| -1.5686 | 1.440188|
| S       | -1.60991| -0.40468| -0.68056|
| C       | -2.16552| -1.53511| 1.553155|
| H       | -0.09774| -1.9598 | 2.210366|
| H       | -2.70493| -1.91175| 2.41746 |
| N       | -8.36399| -0.10852| 0.34633 |
| C       | -8.84999| 1.172013| -0.72204|
| C       | -9.73185| 1.285321| -1.803  |
| C       | -8.46028| 2.310865| -0.01176|
| C       | -10.23  | 2.527434| -2.18545|
| H       | -10.0198| 0.383833| 2.33893 |
| H       | -7.78155| 2.213043| 0.83413 |
| C       | -9.83456| 3.600131| -1.4931 |
| H       | -10.9149| 2.600939| -3.02984|
| C       | -9.29581| -1.16741| -0.20023|
| C       | -10.4911| -0.94325| 0.488857|
| C       | -9.03715| -2.42342| 0.76391 |
| H       | -10.6831| 0.036724| 0.923166|
| C       | -9.95466| -3.46202| -0.63168|
| C       | -11.1429| 3.24076 | 0.04541 |
| H       | -9.73992| 4.43445 | -1.07442|
| C       | -11.4083| 1.97901 | 0.597927|
| C       | -12.7152| -2.02832| 1.251017|
| C       | -12.2853| -4.20133| 0.30859 |
| C       | -8.94946| 3.547891| -0.41019|
| C       | -8.72303| 4.884537| 0.138222|
| C       | -10.2282| 5.104599| -1.72758|
| C       | -9.46453| 5.80338 | -0.61973|
| C       | -9.43341| 7.153193| -0.31084|
| C       | -7.94734| 5.311503| 1.210505|
| C       | -8.65749| 7.582451| 0.765514|
| H       | -10.0075| 7.870513| -0.89709|
| C       | -7.92172| 6.668323| 1.518539|
| H       | -7.37128| 4.599815| 1.799431|
| H       | -8.62567| 8.638987| 1.021206|
| H       | -7.3221 | 7.0198  | 2.354937|
| C       | -13.2392| -3.31966| 1.091698|
| C   | -14.4783 | -3.64301 | 1.619765 |
|-----|----------|----------|----------|
| C   | -13.4279 | -1.05258 | 1.939241 |
| C   | -15.194  | -2.66582 | 2.311148 |
| H   | -14.8898 | -4.64479 | 1.497485 |
| C   | -14.6721 | -1.38246 | 2.468207 |
| H   | -13.0214 | -0.05019 | 2.06287  |
| H   | -16.168  | -2.90523 | 2.731624 |
| H   | -15.2437 | -0.63236 | 3.009785 |
| C   | -9.7682  | 5.587031 | -3.10545 |
| H   | -8.68767 | 5.451392 | -3.22722 |
| H   | -10.2766 | 5.02857  | -3.90158 |
| H   | -9.9977  | 6.651544 | -3.2405  |
| C   | -11.7378 | 5.302619 | -1.57598 |
| H   | -12.0035 | 6.361835 | -1.68364 |
| H   | -12.2807 | 4.739523 | -2.34567 |
| H   | -12.082  | 4.960648 | -0.59351 |
| C   | -11.8244 | -5.39876 | 1.142808 |
| H   | -11.0837 | -5.99239 | 0.592038 |
| H   | -11.3693 | -5.06913 | 2.083629 |
| H   | -12.6711 | -6.05434 | 1.382572 |
| C   | -12.9206 | -4.68256 | -0.99802 |
| H   | -12.2009 | -5.26577 | -1.58653 |
| H   | -13.7882 | -5.32334 | -0.7952  |
| H   | -13.2553 | -3.83497 | -1.60662 |
| C   | 12.57053 | 1.867994 | 0.826562 |
| C   | 13.87097 | 1.505933 | 0.442933 |
| C   | 14.93761 | 2.369346 | 0.678682 |
| C   | 14.66132 | 3.580413 | 1.29593  |
| C   | 13.37307 | 3.949297 | 1.679469 |
| C   | 12.3146  | 3.078794 | 1.441495 |
| C   | 11.62471 | 0.791636 | 0.476863 |
| C   | 12.4278  | -0.27047 | -0.15626 |
| C   | 13.81785 | 0.164751 | -0.18215 |
| H   | 15.96659 | 2.155031 | 0.41229  |
| O   | 10.42417 | 0.794575 | 0.678956 |
| C   | 14.91572 | -0.49943 | -0.68166 |
| C   | 16.23454 | 0.041435 | -0.65246 |
| N   | 17.32091 | 0.460169 | -0.64208 |
| C   | 14.85595 | -1.79183 | -1.28121 |
| N   | 14.82799 | -2.84669 | -1.77407 |
| H   | -8.1077  | -2.57531 | -1.30785 |
| F   | 15.64156 | 4.435788 | 1.540501 |
| F   | 13.16225 | 5.115788 | 2.262666 |
| C   | -4.21707 | -0.72099 | 0.265202 |
### Table S6: Cartesian coordinates of MCPTD5

| Atom | X-axis  | Y-axis  | Z-axis  |
|------|---------|---------|---------|
| C    | -6.12326| -4.55365| 0.020523|
| C    | -4.80896| -4.84749| -0.27616|
| C    | -3.8175 | -3.86696| -0.16561|
| C    | -4.17443| -2.56677| 0.283087|
| C    | -5.33164| -2.26895| 0.61501 |
| C    | -6.51718| -3.27667| 0.450624|
| C    | -2.45234| -4.14581| -0.47159|
| C    | -3.16197| -1.56833| 0.401976|
| C    | -1.81313| -1.85477| 0.034921|
| C    | -1.49539| -3.1886 | -0.37638|
| C    | -0.8363 | -0.83222| 0.126507|
| C    | -1.20676| 0.417327 | 0.642652|
| C    | -2.50569| 0.687539 | 1.024674|
| C    | -3.50394| -0.2833 | 0.89866 |
| C    | -4.85356| -0.02796| 1.278704|
| C    | -5.82037| -0.97115| 1.147391|
| H    | -6.82919| -0.74314| 1.47558 |
| H    | -5.09551| 0.949084 | 1.693422|
| H    | -2.19061| -5.15864| -0.77305|
| H    | -6.88694| -5.31504| -0.12048|
| H    | -4.53393| -5.84287| -0.61977|
| H    | -0.45901| -3.43353| -0.58965|
| H    | -0.45267| 1.198929 | 0.70886 |
| H    | -2.76976| 1.670292 | 1.411143|
| C    | -11.6475| -1.80797| 0.673229|
| H    | -12.3593| -2.51491 | 1.095754|
| C    | -10.3422| -2.35375| 0.707784|
| C    | -10.1273| -3.61948 | 1.256514|
| S    | -8.81874| -1.67564| 0.15943 |
| C    | -8.79784| -4.02863 | 1.24227 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | -10.9477| -4.20522| 1.66372 |
| C       | -7.94648| -3.08278| 0.687035|
| H       | -8.44196| -4.97116| 1.646474|
| C       | 0.544949| -1.03115| -0.31101 |
| C       | 1.028828| -1.58258| -1.47196 |
| S       | 1.866383| -0.43926| 0.666411 |
| C       | 2.43645 | -1.52215| -1.58739 |
| H       | 0.374585| -1.97335| 2.322598 |
| H       | 2.980563| -1.8745 | -2.45895 |
| N       | 8.617616| -0.05332| 0.331456 |
| C       | 9.093646| 1.224401| 0.727915 |
| C       | 9.981481| 1.326592| 1.805182 |
| C       | 8.687893| 2.372611| 0.041863 |
| C       | 10.46906| 2.56644 | 2.208101 |
| H       | 10.28219| 0.418263| 2.322598 |
| H       | 8.005164| 2.283989| -0.8018  |
| C       | 10.05677| 3.708049| 1.540773 |
| H       | 11.15832| 2.631073| 3.049641 |
| C       | 9.55612 | -1.10472| 0.172068 |
| C       | 10.74574| -0.86814| -0.52235 |
| C       | 9.30729 | -2.3665 | 0.726966 |
| H       | 10.92975| 0.116327| -0.94992 |
| C       | 10.22922| -3.39927| 0.580777 |
| C       | 11.41198| -3.16596| -0.10186 |
| H       | 10.02246| -4.37647| 1.016769 |
| C       | 11.66758| -1.89833| -0.64567 |
| C       | 12.97087| -1.93554| -1.30684 |
| C       | 12.55783| -4.11827| -0.3793  |
| C       | 9.166176| 3.60929 | 0.461275 |
| C       | 8.921125| 4.95135 | -0.05919 |
| C       | 10.43496| 5.151998| 1.801727 |
| C       | 9.656376| 5.863663| 0.712583 |
| C       | 9.607641| 7.218845| 0.430981 |
| C       | 8.134111| 5.390411| -1.11828 |
| C       | 8.820226| 7.660334| -0.63202 |
| H       | 10.17718| 7.93074 | 1.028158 |
| C       | 8.090736| 6.752695| -1.39892 |
| H       | 7.562807| 4.683917| -1.71801 |
| H       | 8.774512| 8.721304| -0.86635 |
| H       | 7.481973| 7.113746| -2.22456 |
| C       | 13.50235| -3.22538| -1.16085 |
| C       | 14.74044| -3.53788| -1.69768 |
| C       | 13.67508| -0.95057| -1.9907  |
| C       | 15.4477 | -2.55138| -2.38443 |
|   |   |   |
|---|---|---|
| H | 15.15778 | -4.53842 | -1.58531 |
| C | 14.91843 | -1.26955 | -2.52854 |
| H | 13.26286 | 0.050721 | -2.10405 |
| H | 16.42089 | -2.78217 | -2.81149 |
| H | 15.48333 | -0.51199 | -3.0667 |
| C | 9.97807 | 5.60146 | 3.19177 |
| H | 8.899756 | 5.451837 | 3.316945 |
| H | 10.49701 | 6.665448 | 3.347166 |
| C | 11.94113 | 5.371336 | 1.644937 |
| H | 12.19474 | 6.431291 | 1.772857 |
| H | 12.49577 | 4.799175 | 2.399418 |
| H | 12.28322 | 5.053961 | 0.653496 |
| C | 12.09874 | -5.31192 | -1.21981 |
| H | 11.36491 | -5.914 | -0.66909 |
| H | 11.63613 | -4.97782 | -2.15537 |
| H | 12.94781 | -5.96073 | -1.46953 |
| C | 13.20364 | -4.60562 | 0.919943 |
| H | 12.49084 | -5.19734 | 1.508355 |
| H | 14.07367 | -5.2398 | 0.707214 |
| H | 13.53704 | -3.76066 | 1.532866 |
| C | -12.3668 | 1.556303 | -0.66565 |
| C | -13.651 | 1.155624 | -0.28087 |
| C | -14.7169 | 2.029523 | -0.47522 |
| C | -14.4644 | 3.277042 | -1.04578 |
| C | -13.1679 | 3.659977 | -1.42409 |
| C | -12.1038 | 2.785735 | -1.23194 |
| C | -11.4 | 0.48259 | -0.36971 |
| C | -12.1718 | -0.61749 | 0.233062 |
| C | -13.5724 | -0.2087 | 0.287188 |
| H | -15.7392 | 1.787416 | -0.2039 |
| O | -10.2019 | 0.528288 | -0.59205 |
| C | -14.6536 | -0.91427 | 0.763995 |
| C | -15.9802 | -0.39166 | 0.76495 |
| N | -17.0721 | 0.012107 | 0.778299 |
| C | -14.568 | -2.23081 | 1.305406 |
| N | -14.5179 | -3.30557 | 1.751244 |
| H | 8.381386 | -2.52727 | 1.27445 |
| C | 4.477186 | -0.70014 | -0.28853 |
| C | 4.937723 | 0.247427 | 0.635043 |
| C | 5.442237 | -1.42954 | -0.99692 |
| C | 6.288682 | 0.453475 | 0.850213 |
| H | 4.221188 | 0.841918 | 1.200111 |
| C | 6.795438 | -1.21294 | -0.80868 |
| Atom | X-axis | Y-axis | Z-axis |
|------|--------|--------|--------|
| C    | -5.7301| -4.603 | -0.12352|
| C    | -4.41442| -4.8671| -0.44041|
| C    | -3.44136| -3.86801| -0.3314|
| C    | -3.81987| -2.57747| 0.126933|
| C    | -5.17973| -2.30779| 0.472341|
| C    | -6.14457| -3.33758| 0.321531|
| C    | -2.07308| -4.12056| -0.64575|
| C    | -2.82467| -1.56161| 0.247044|
| C    | -1.47145| -1.82362| -0.12169|
| C    | -1.13206| -3.14834| -0.54462|
| C    | -0.51035| -0.7875| -0.01842|
| C    | -0.90076| 0.452973| 0.504147|
| C    | -2.20516| 0.701059| 0.883087|
| C    | -3.18744| -0.28532| 0.751025|
| C    | -4.54059| -0.05493| 1.134457|
| C    | -5.49012| -1.01607| 1.007074|
| H    | -6.50134| -0.80632| 1.339772|
| H    | -4.79955| 0.917242| 1.550323|
| H    | -1.79531| -5.12629| -0.95643|
| H    | -6.4795| -5.37998| -0.25583|
| H    | -4.12296| -5.85419| -0.79421|
| H    | -0.09219| -3.37392| -0.76222|
| H    | -0.15753| 1.244173| 0.579035|
| H    | -2.48585| 1.677206| 1.274533|
| C    | -11.3036| -2.0268| 0.787124|
| H    | -11.961| -2.75811| 1.252717|
| C    | -9.98328| -2.53101| 0.740338|
| C    | -9.70326| -3.78929| 1.278211|
| S    | -8.50984| -1.80859| 0.116922|
| C    | -8.36482| -4.15742| 1.200464|
| H    | -10.4846| -4.39711| 1.728138|
| C    | -7.5701| -3.18555| 0.606193|
| H    | -7.96107| -5.08642| 1.590528|

Table S7: Cartesian coordinates of MCPTD6
|  |  |  |  |
|---|---|---|---|
| C | 0.877088 | -0.96752 | -0.44525 |
| C | 1.377176 | -1.49506 | -1.61025 |
| S | 2.183574 | -0.39463 | 0.562596 |
| C | 2.786422 | -1.43231 | -1.70409 |
| H | 0.733936 | -1.87201 | -2.40069 |
| H | 3.344406 | -1.76713 | -2.57384 |
| N | 8.942215 | -0.05035 | 0.351589 |
| C | 9.425792 | 1.221199 | 0.758973 |
| C | 10.29235 | 1.311688 | 1.854365 |
| C | 9.049547 | 2.374518 | 0.064717 |
| C | 10.78881 | 2.544915 | 2.266675 |
| H | 10.57017 | 0.39961 | 2.37794 |
| H | 8.383333 | 2.294863 | -0.79289 |
| C | 10.40665 | 3.691565 | 1.59014 |
| H | 11.46136 | 2.600212 | 3.122251 |
| C | 9.871683 | -1.11162 | 0.2061 |
| C | 11.07974 | -0.88409 | -0.459 |
| C | 9.596566 | -2.37449 | 0.746299 |
| H | 11.2845 | 0.101035 | -0.87543 |
| C | 10.51031 | -3.41633 | 0.613966 |
| C | 11.7113 | -3.19187 | -0.03932 |
| H | 10.28234 | -4.39394 | 1.038298 |
| C | 11.99318 | -1.92334 | -0.5677 |
| C | 13.31126 | -1.96999 | -1.19786 |
| C | 12.85326 | -4.15458 | -0.2966 |
| C | 9.536564 | 3.602388 | 0.49304 |
| C | 9.322241 | 4.949719 | -0.03342 |
| C | 10.80164 | 5.129942 | 1.85705 |
| C | 10.05622 | 5.851759 | 0.751542 |
| C | 10.03434 | 7.207052 | 0.467084 |
| C | 8.563159 | 5.399211 | -1.10843 |
| C | 9.275247 | 7.658909 | -0.61202 |
| H | 10.60302 | 7.91105 | 1.074338 |
| C | 8.546781 | 6.761499 | -1.39189 |
| H | 7.992532 | 4.700718 | -1.71811 |
| H | 9.250775 | 8.720035 | -0.84883 |
| H | 7.960104 | 7.13061 | -2.22985 |
| C | 13.82642 | -3.26597 | -1.0476 |
| C | 15.07338 | -3.58765 | -1.55791 |
| C | 14.04023 | -0.9881 | -1.85974 |
| C | 15.80558 | -2.60418 | -2.22267 |
| H | 15.47807 | -4.59302 | -1.44254 |
| C | 15.29212 | -1.31642 | -2.3712 |
| H | 13.6402 | 0.017673 | -1.97676 |
|   |       |       |       |
|---|-------|-------|-------|
| H | 16.78584 | -2.84222 | -2.62909 |
| H | 15.87634 | -0.5617 | -2.89247 |
| C | 10.32377 | 5.588228 | 3.237123 |
| H | 9.24114 | 5.454602 | 3.341192 |
| H | 10.81886 | 5.012851 | 4.029623 |
| H | 10.55539 | 6.649063 | 3.395627 |
| C | 12.31393 | 5.32555 | 1.730926 |
| H | 12.5815 | 6.381611 | 1.862432 |
| H | 12.84399 | 4.746292 | 2.497579 |
| H | 12.67144 | 5.001015 | 0.747269 |
| C | 12.40179 | -5.33539 | -1.15914 |
| H | 11.64636 | -5.93267 | -0.63297 |
| H | 11.96781 | -4.98746 | -2.10335 |
| H | 13.24906 | -5.99256 | -1.3925 |
| C | 13.4606 | -4.66071 | 1.013878 |
| H | 12.72618 | -5.24872 | 1.578963 |
| H | 14.32801 | -5.30357 | 0.817364 |
| H | 13.78857 | -3.82516 | 1.642408 |
| C | -12.2429 | 1.304647 | -0.51723 |
| C | -13.4752 | 0.853349 | -0.02018 |
| C | -14.6006 | 1.661106 | -0.11224 |
| C | -14.4741 | 2.913042 | -0.70786 |
| C | -13.2503 | 3.372494 | -1.21515 |
| C | -12.1163 | 2.549776 | -1.11413 |
| C | -11.2146 | 0.260792 | -0.27847 |
| C | -11.9034 | -0.8567 | 0.389015 |
| C | -13.3037 | -0.50153 | 0.550035 |
| H | -15.5748 | 1.363401 | 0.258986 |
| O | -10.0356 | 0.316181 | -0.5749 |
| C | -14.3165 | -1.24179 | 1.118732 |
| C | -15.6628 | -0.78453 | 1.223097 |
| N | -16.7709 | -0.44168 | 1.324619 |
| C | -14.1327 | -2.5461 | 1.665675 |
| N | -14.0045 | -3.61177 | 2.117774 |
| H | 8.657053 | -2.52933 | 1.27182 |
| C | 4.808565 | -0.64571 | -0.35651 |
| C | 5.260587 | 0.293251 | 0.579862 |
| C | 5.779246 | -1.38272 | -1.04899 |
| C | 6.6093 | 0.483187 | 0.82295 |
| H | 4.539221 | 0.893491 | 1.132585 |
| C | 7.130732 | -1.1823 | -0.83253 |
| H | 5.467056 | -2.13468 | -1.77072 |
| C | 7.572091 | -0.24863 | 0.115822 |
| H | 6.929067 | 1.210857 | 1.56462 |
Table S8: Cartesian coordinates of MCPTD7

| Atom | X-axis  | Y-axis  | Z-axis  |
|------|---------|---------|---------|
| C    | 6.358431| -4.43185| -0.00862|
| C    | 5.047294| -4.73741| 0.285814|
| C    | 4.0485  | -3.76267| 0.183334|
| C    | 4.395786| -2.45556| -0.25344|
| C    | 5.751039| -2.14368| -0.58083|
| C    | 6.744196| -3.14674| -0.42533|
| C    | 2.685896| -4.05574| 0.484616|
| C    | 3.375315| -1.46489| -0.36564|
| C    | 2.028194| -1.76607| -0.00449|
| C    | 1.721027| -3.10562| 0.394399|
| C    | 1.049156| -0.75183| -0.09084|
| C    | 1.40273 | 0.505253| -0.59624|
| C    | 2.700183| 0.790147| -0.97186|
| C    | 3.706901| -0.17294| -0.85092|
| C    | 5.05439 | 0.096819| -1.2264 |
| C    | 6.02927 | -0.83958| -1.10168|
| H    | 7.035602| -0.59969| -1.42886|
| H    | 5.288916| 1.079041| -1.63301|
| H    | 2.431984| -5.07317| 0.776804|
| H    | 7.126321| -5.18969| 0.127584|
| H    | 4.779465| -5.73753| 0.620887|
| H    | 0.686246| -3.36144| 0.6022 |
| H    | 0.641948| 1.280554| -0.65882|
| H    | 2.956398| 1.778361| -1.34949|
| C    | 11.8632 | -1.65473| -0.625 |
| H    | 12.58169| -2.36346| -1.03278|
| C    | 10.56413| -2.20179| -0.66615|
| C    | 10.35855| -3.47806| -1.20122|
| S    | 9.031307| -1.52418| -0.13846|
| C    | 9.03414 | -3.89278| -1.19107|
| H    | 11.18512| -4.06485| -1.59435|
| C    | 8.171322| -2.94316| -0.65274|
| H    | 8.686062| -4.84123| -1.58755|
| C    | -0.33888| -0.96759| 0.338333|
| C    | -0.82328| -1.53692| 1.490636|
| S    | -1.66096| -0.37716| -0.6392 |
|     |    X   |    Y   |    Z   |
|-----|--------|--------|--------|
|   C | -2.23178 | -1.49164 | 1.599255 |
|   H | -0.16958  | -1.92915 | 2.264788  |
|   H | -2.77746  | -1.85902 | 2.463562  |
|   N | -8.41616  | -0.07413 | -0.34538  |
|   C | -8.90517  | 1.203012 | -0.72973  |
|   C | -9.77923  | 1.307549 | -1.81769  |
|   C | -8.52769  | 2.346146 | -0.01973  |
|   C | -10.2817  | 2.545574 | -2.20776  |
|   H | -10.058   | 0.402465 | -2.35286  |
|   H | -7.85565  | 2.255008 | 0.832212  |
|   C | -9.89841  | 3.682598 | -1.51576  |
|   H | -10.9605  | 2.612383 | -3.05755  |
|   C | -9.34641  | -1.13527 | -0.20042  |
|   C | -10.541   | -0.91421 | 0.49054   |
|   C | -9.08636  | -2.38915 | -0.7678   |
|   H | -10.7337  | 0.064713 | 0.926952  |
|   C | -10.0021  | -3.42953 | -0.63693  |
|   C | -11.1897  | -3.21162 | 0.042473  |
|   H | -9.78667  | -4.4006  | -1.0823   |
|   C | -11.4565  | -1.95169 | 0.598556  |
|   C | -12.7622  | -2.00502 | 1.253667  |
|   C | -12.3299  | -4.17487 | 0.305091  |
|   C | -9.02105  | 3.579107 | -0.42568  |
|   C | -8.80731  | 4.918716 | 0.12049   |
|   C | -10.2995  | 5.123821 | -1.75737  |
|   C | -9.54875  | 5.830606 | -0.64584  |
|   C | -9.52866  | 7.181456 | -0.34058  |
|   C | -8.04278  | 5.353593 | 1.197624  |
|   C | -8.76398  | 7.618634 | 0.740588  |
|   H | -10.1028  | 7.893417 | -0.93326  |
|   C | -8.0283   | 6.711367 | 1.502025  |
|   H | -7.46679  | 4.647285 | 1.793076  |
|   H | -8.74086  | 8.676044 | 0.993548  |
|   H | -7.43756  | 7.06908  | 2.342064  |
|   C | -13.284   | -3.29697 | 1.092137  |
|   C | -14.5214  | -3.62401 | 1.62178   |
|   C | -13.4753  | -1.0323  | 1.945676  |
|   C | -15.2376  | -2.64989 | 2.317011  |
|   H | -14.9313  | -4.62624 | 1.497873  |
|   C | -14.7179  | -1.36591 | 2.476245  |
|   H | -13.0705  | -0.02945 | 2.071006  |
|   H | -16.2102  | -2.89223 | 2.738816  |
|   H | -15.2898  | -0.6183  | 3.020808  |
|   C | -9.83268  | 5.60513  | -3.1333   |
|    | XYZ    |   | XYZ    |
|----|--------|---|--------|
| H  | -8.75048 | 5.47601 | -3.24706 |
| H  | -10.332   | 5.04119 | -3.93133 |
| H  | -10.068   | 6.66734 | -3.27312 |
| C  | -11.8115  | 5.312315 | -1.61749 |
| H  | -12.083   | 6.369444 | -1.73014 |
| H  | -12.3451  | 4.743604 | -2.38957 |
| H  | -12.1609  | 4.970911 | -0.63662 |
| C  | -11.8653  | -5.37367 | 1.135322 |
| H  | -11.1247  | -5.96471 | 0.581618 |
| H  | -11.409   | -5.04577 | 2.076175 |
| H  | -12.7104  | -6.03125 | 1.374981 |
| C  | -12.9665  | -4.65384 | -1.00172 |
| H  | -12.2469  | -5.23454 | -1.59282 |
| H  | -13.8327  | -5.29644 | -0.79901 |
| H  | -13.3035  | -3.80532 | -1.60771 |
| C  | 12.56774  | 1.72445  | 0.697672 |
| C  | 13.85701  | 1.320466 | 0.333574 |
| C  | 14.92281  | 2.192509 | 0.537864 |
| C  | 14.66409  | 3.447882 | 1.098942 |
| C  | 13.35409  | 3.837513 | 1.457207 |
| C  | 12.2914   | 2.956321 | 1.252215 |
| C  | 11.60364  | 0.644073 | 0.393144 |
| C  | 12.38312  | -0.45576 | -0.1887 |
| C  | 13.78185  | -0.05023 | -0.22869 |
| H  | 15.94731  | 1.943191 | 0.281519 |
| O  | 10.40369  | 0.699368 | 0.600657 |
| C  | 14.8714   | -0.75495 | -0.68699 |
| C  | 16.19761  | -0.23165 | -0.67368 |
| N  | 17.28864  | 0.174401 | -0.6743 |
| C  | 14.79247  | -2.07421 | -1.22308 |
| N  | 14.74502  | -3.15102 | -1.66381 |
| H  | -8.15729  | -2.538   | -1.3133 |
| C  | -4.27349  | -0.67729 | 0.297088 |
| C  | -4.73934  | 0.282674 | -0.61089 |
| C  | -5.23406  | -1.43407 | 0.982517 |
| C  | -6.091    | 0.474982 | -0.83293 |
| H  | -4.02641  | 0.898456 | -1.15742 |
| C  | -6.58845  | -1.23261 | 0.786975 |
| H  | -4.91176  | -2.20215 | 1.682524 |
| C  | -7.04392  | -0.2764 | -0.13227 |
| H  | -6.42098  | 1.219693 | -1.55271 |
| H  | -7.30921  | -1.82588 | 1.344004 |
| C  | -2.8506   | -0.88957 | 0.53008 |
| H  | 11.27227  | 3.225011 | 1.518126 |
| Atom | X-axis  | Y-axis  | Z-axis  |
|------|---------|---------|---------|
| C    | -6.20941| -4.35579| -0.25549|
| C    | -4.89625| -4.62648| -0.57923|
| C    | -3.91673| -3.6346 | -0.46834|
| C    | -4.28574| -2.34427| -0.00187|
| C    | -5.64264| -2.06856| 0.350198|
| C    | -6.61399| -3.09132| 0.199536|
| C    | -2.55085| -3.89366| -0.78908|
| C    | -3.28392| -1.33527| 0.120796|
| C    | -1.93307| -1.60424| -0.25198|
| C    | -1.6033 | -2.92845| -0.68508|
| C    | -0.96492| -0.57582| -0.14225|
| C    | -1.34579| 0.664475| 0.386858|
| C    | -2.64843| 0.919939| 0.767875|
| C    | -3.63737| -0.05911| 0.632352|
| C    | -4.98881| 0.178073| 1.019562|
| C    | -5.94424| -0.77669| 0.890607|
| H    | -6.95438| -0.56305| 1.22456|
| H    | -5.24054| 1.150227| 1.439999|
| H    | -2.28066| -4.89918| -1.10728|
| H    | -6.96449| -5.12739| -0.3872 |
| H    | -4.6124 | -5.61367| -0.93909|
| H    | -0.56569| -3.15891| -0.90823|
| H    | -0.596  | 1.449129| 0.466589|
| H    | -2.92185| 1.895818| 1.165178|
| C    | -11.77 | -1.7677 | 0.700573|
| H    | -12.4264| -2.49499| 1.173966|
| C    | -10.4475| -2.27488| 0.650768|
| C    | -10.165 | -3.52747| 1.195403|
| S    | -8.98028| -1.55814| 0.008174|
| C    | -8.82596| -3.89842| 1.108104|
| H    | -10.9434| -4.13085| 1.655992|
| C    | -8.03731| -2.93365| 0.498765|
| H    | -8.41996| -4.8256 | 1.500545|
| C    | 0.422506| -0.76544| -0.56681|
| C    | 0.921022| -1.28096| -1.73757|
| S    | 1.731048| -0.23107| 0.458702|
| C    | 2.331884| -1.23966| -1.82157|

Table S9: Cartesian coordinates of MCPTD8
|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| H   | 0.276527  | -1.63569  | -2.53725  |
| H   | 2.89072   | -1.56929  | -2.69281  |
| N   | 8.498433  | -0.0331   | 0.311337  |
| C   | 9.011883  | 1.234245  | 0.692222  |
| C   | 9.870308  | 1.332642  | 1.793651  |
| C   | 8.668463  | 2.378571  | -0.0332   |
| C   | 10.39304  | 2.563915  | 2.178346  |
| H   | 10.12218  | 0.428355  | 2.343084  |
| H   | 8.007547  | 2.292896  | -0.89441  |
| C   | 10.04421  | 3.701827  | 1.469627  |
| H   | 11.05992  | 2.624807  | 3.038021  |
| C   | 9.387262  | -1.13325  | 0.224082  |
| C   | 10.64364  | -0.96478  | -0.36525  |
| C   | 9.020599  | -2.38225  | 0.742853  |
| H   | 10.92348  | 0.00823   | -0.76575  |
| C   | 9.888196  | -3.46772  | 0.661967  |
| C   | 11.13594  | -3.30205  | 0.083334  |
| H   | 9.585646  | -4.43287  | 1.067902  |
| C   | 11.51045  | -2.04746  | -0.42015  |
| C   | 12.8639   | -2.15558  | -0.96249  |
| C   | 12.24328  | -4.31835  | -1.0761   |
| C   | 9.180257  | 3.605192  | 0.368501  |
| C   | 9.000057  | 4.943608  | -0.19249  |
| C   | 10.47331  | 5.13668   | 1.701532  |
| C   | 9.749667  | 5.84792   | 0.574871  |
| C   | 9.75942   | 7.196111  | 0.257478  |
| C   | 8.257035  | 5.38346   | -1.28259  |
| C   | 9.016255  | 7.638266  | -0.83661  |
| H   | 10.33988  | 7.902245  | 0.850973  |
| C   | 8.272333  | 6.73852   | -1.59895  |
| H   | 7.674326  | 4.68305   | -1.87846  |
| H   | 9.01614   | 8.693707  | -1.0988   |
| H   | 7.69838   | 7.099988  | -2.44899  |
| C   | 13.30626  | -3.47521  | -0.78579  |
| C   | 14.56977  | -3.85245  | -1.20969  |
| C   | 13.68275  | -1.20611  | -1.56375  |
| C   | 15.39262  | -2.90106  | -1.8122   |
| H   | 14.91909  | -4.87602  | -1.07503  |
| C   | 14.95149  | -1.5899   | -1.98682  |
| H   | 13.33984  | -0.18186  | -1.69971  |
| H   | 16.38755  | -3.18303  | -2.1489   |
| H   | 15.60691  | -0.86099  | -2.45779  |
| C   | 10.00366  | 5.641865  | 3.067765  |
| H   | 8.918018  | 5.536342  | 3.172496  |
|  | X  | Y  | Z   |
|---|----|----|-----|
| H | 10.48369 | 5.075652 | 3.875977 |
| H | 10.26003 | 6.700653 | 3.199325 |
| C | 11.99033 | 5.291359 | 1.574894 |
| H | 12.28385 | 6.343498 | 1.679946 |
| H | 12.50416 | 4.718854 | 2.357516 |
| H | 12.34149 | 4.932913 | 0.600754 |
| C | 11.7907 | -5.47053 | -1.00758 |
| H | 10.97533 | -6.03232 | -0.53434 |
| H | 11.43376 | -5.09605 | -1.97363 |
| H | 12.61766 | -6.16754 | -1.19335 |
| C | 12.73907 | -4.86114 | 1.234678 |
| H | 11.94158 | -5.41366 | 1.747583 |
| H | 13.5836 | -5.54641 | 0.48754 |
| H | 13.06782 | -4.04627 | 1.889416 |
| C | -12.6828 | 1.563375 | -0.59974 |
| C | -13.9377 | 1.11806 | -0.1019 |
| C | -15.0327 | 1.944894 | -0.20418 |
| C | -14.8903 | 3.221392 | -0.80478 |
| C | -13.6207 | 3.652201 | -1.3034 |
| C | -12.509 | 2.783672 | -1.18517 |
| C | -11.6697 | 0.52063 | -0.37145 |
| C | -12.3619 | -0.59848 | 0.296919 |
| C | -13.7682 | -0.23625 | 0.458754 |
| H | -16.0156 | 1.660294 | 0.159092 |
| O | -10.4903 | 0.584117 | -0.68019 |
| C | -14.7809 | -0.98324 | 1.02291 |
| C | -16.1234 | -0.51504 | 1.12576 |
| N | -17.2273 | -0.15727 | 1.223137 |
| C | -14.6044 | -2.29176 | 1.559735 |
| N | -14.4804 | -3.36178 | 2.003626 |
| H | 8.043271 | -2.49142 | 1.207433 |
| C | 4.35826 | -0.51437 | -0.44761 |
| C | 4.82354 | 0.407514 | 0.499153 |
| C | 5.317016 | -1.26974 | -1.13713 |
| C | 6.174401 | 0.561158 | 0.75713 |
| H | 4.111607 | 1.021677 | 1.048696 |
| C | 6.67074 | -1.10438 | -0.90565 |
| H | 4.992803 | -2.00838 | -1.86728 |
| C | 7.12479 | -0.19111 | 0.055789 |
| H | 6.505923 | 1.275295 | 1.50693 |
| H | 7.391799 | -1.69604 | -1.4641 |
| C | 2.936453 | -0.69558 | -0.71449 |
| H | -11.5271 | 3.079576 | -1.55188 |
| C | -13.5145 | 4.930636 | -1.89703 |
Table S10: Calculated energies (E) and energy gap (ΔE) for MCPTR, MCPTD1, MCPTD2, MCPTD3, MCPTD4, MCPTD5, MCPTD6, MCPTD7 and MCPTD8.

| System  | $E_{\text{HOMO}-1}$ | $E_{\text{LUMO}-1}$ | ΔE  | $E_{\text{HOMO}-2}$ | $E_{\text{LUMO}-2}$ | ΔE  |
|---------|---------------------|---------------------|------|---------------------|---------------------|------|
| MCPTR   | -6.667              | -1.648              | 5.019| -6.955              | -0.819              | 6.136|
| MCPTD1  | -5.698              | -1.847              | 3.851| -6.212              | -1.057              | 5.155|
| MCPTD2  | -5.687              | -2.418              | 3.269| -6.214              | -1.909              | 4.305|
| MCPTD3  | -5.719              | -2.520              | 3.199| -6.229              | -1.930              | 4.299|
| MCPTD4  | -5.722              | -2.569              | 3.153| -6.229              | -1.936              | 4.293|
| MCPTD5  | -5.726              | -2.627              | 3.099| -6.230              | -1.960              | 4.270|
| MCPTD6  | -5.734              | -2.703              | 3.780| -6.229              | -1.974              | 4.255|
| MCPTD7  | -5.762              | -3.089              | 2.673| -6.236              | -2.072              | 4.164|
| MCPTD8  | -5.704              | -2.304              | 3.400| -6.221              | -1.947              | 4.274|

$E$ = energy, $\Delta E (eV) = E_{\text{LUMO}} - E_{\text{HOMO}}$; HOMO = highest occupied molecular orbital; LUMO = lowest unoccupied molecular orbital, MO, molecular orbital

Table S11: Dipole moments, dipole polarizability and major contributing tensor (a.u) of (MCPTR – MCPTD8).

| System  | $\alpha_{xx}$ | $\alpha_{yy}$ | $\alpha_{zz}$ | $\mu_x$  | $\mu_y$  | $\mu_z$  |
|---------|----------------|----------------|----------------|-----------|-----------|-----------|
| MCPTR   | 868.3          | 564.5          | 244.6          | -0.669    | -2.910    | -1.848    |
| MCPTD1  | 1967.8         | 1239.7         | 715.8          | 1.052     | -2.880    | 1.556     |
| MCPTD2  | 2339.5         | 1007.5         | 1081.0         | -4.031    | 0.561     | -0.268    |
| MCPTD3  | 2430.9         | 1379.5         | 696.0          | -4.715    | 0.422     | 0.422     |
| MCPTD4  | 2473.9         | 1386.2         | 686.5          | -4.341    | 0.778     | -0.052    |
| MCPTD5  | 2518.8         | 1472.2         | 699.3          | -4.950    | -0.701    | 0.154     |
| MCPTD6  | 2560.5         | 1471.1         | 718.2          | -4.605    | -0.746    | 0.189     |
| MCPTD7  | 2668.8         | 1493.9         | 700.2          | -6.337    | -3.325    | -0.792    |
| MCPTD8  | 2509.3         | 1563.6         | 716.7          | -3.860    | 1.232     | 0.95      |

Table S12: The computed first-order hyperpolarizabilities ($\beta_{101}$) and major contributing tensors (a.u) of the studied compounds (MCPTR – MCPTD8).

| Compound | $\beta_{xx}$ | $\beta_{yy}$ | $\beta_{zz}$ | $\beta_{xy}$ | $\beta_{xz}$ | $\beta_{yz}$ | $\beta_{xxy}$ | $\beta_{xzz}$ | $\beta_{xz}$ | $\beta_{yz}$ |
|----------|--------------|--------------|--------------|--------------|--------------|--------------|---------------|--------------|--------------|--------------|
| MCPTR    | -23469.6    | -1493.0      | 491.0        | 343.8        | -2612.2      | 95.6         | -268.1        | 60.7         | 12.0         |
| MCPTD1   | 74202.8     | -2823.4      | -948.3       | -674.2       | -829.9       | -384.6       | 145.7         | 130.2        | -55.9        |
| MCPTD2   | -145431     | 16235.8      | -2046.2      | 884.9        | 16526.6      | 157.6        | -3473.1       | -552.8       | 538.2        |
| MCPTD3   | -190677     | 15355.4      | -1103.0      | -1658.1      | -578.5       | -1741.3      | 494.6         | 531.0        | -257.0       |
| MCPTD4   | -213956     | 15659.2      | -1185.1      | -1614.1      | -1702.9      | -1611.3      | 432.4         | -382.3       | -164.2       |
| MCPTD5   | -221413     | -14432.4     | -578.0       | 3673.8       | 2347.7       | 2292.9       | 490.4         | 567.8        | 238.0        |
| MCPTD6   | -234466     | -10854       | 440.3        | 3055.4       | 7854.0       | 2005.1       | 227.8         | 325.9        | 136.5        |
Table S13: Second order hyper polarizability $\gamma$ and major contributing tensor $\gamma$ (a.u.) of the studied compounds (MCPTD – MCPTD8).

| Systems   | $\gamma_x$ | $\gamma_y$ | $\gamma_z$ | $\gamma$ |
|-----------|------------|------------|------------|---------|
| MCPTD1    | 2.0926×10⁶ | 3.4699×10⁴ | 1.7853×10⁴ | 2.1452×10⁶ |
| MCPTD2    | 1.2703×10⁷ | 4.1332×10⁵ | 9.2633×10⁴ | 1.3209×10⁷ |
| MCPTD3    | 4.0204×10⁷ | 8.0632×10⁵ | 9.4683×10⁴ | 4.7632×10⁷ |
| MCPTD4    | 4.6731×10⁷ | 8.0632×10⁵ | 9.4683×10⁴ | 4.7632×10⁷ |
| MCPTD5    | 4.8823×10⁷ | 9.4374×10⁵ | 1.7328×10⁵ | 4.9960×10⁷ |
| MCPTD6    | 5.2915×10⁷ | 1.0162×10⁥ | 1.2087×10⁵ | 5.4032×10⁷ |
| MCPTD7    | 8.4527×10⁷ | 1.3547×10⁥ | 1.4219×10⁵ | 8.6024×10⁷ |
| MCPTD8    | 4.043×10⁷  | 1.215×10⁥  | 1.640×10⁵  | 4.180×10⁷  |

Table S14: Wave length, excitation energy and oscillator strength of investigated compound (MCPTD).

| NO. | DFT $\lambda$ (nm) | E (eV) | $f$  | MO contributions                                      |
|-----|---------------------|--------|------|-------------------------------------------------------|
| 1   | 481.212(424)a       | 2.577  | 0.619| H→L (99%), H-1→L (68%), H→L+1 (25%), H→L+2 (3%)       |
| 2   | 368.332             | 3.3661 | 0.3682|                                                      |
| 3   | 349.517             | 3.5473 | 0.21 | H-2→L (14%), H-1→L (16%), H→L+1 (57%), H→L+2 (7%)    |
| 4   | 336.858             | 3.6806 | 0.3255| H-2→L (58%), H→L+1 (12%), H→L+2 (12%), H-1→L (8%),   |
|     |                     |        |      | H-1→L+1 (3%), H-1→L+2 (2%)                           |
| 5   | 315.795             | 3.9261 | 0.0039| H-2→L (24%), H-1→L+1 (23%), H→L+2 (38%), H-2→L+1 (6%)|
| 6   | 297.788             | 4.1635 | 0.0196| H-2→L (24%), H-1→L+1 (23%), H→L+2 (38%), H-2→L+1 (6%)|

MO=molecular orbital, H=HOMO, L=LUMO, $f$= oscillator strength

Table S15: Wave length, excitation energy and oscillator strength of investigated compound (MCPTD1).

| NO. | DFT $\lambda$ (nm) | E (eV) | $f$  | MO contributions                                      |
|-----|---------------------|--------|------|-------------------------------------------------------|
| 1   | 547.050             | 2.2664 | 0.07388| H-1→L (15%), H→L (82%) H→L+1 (2%)                    |
| 2   | 470.168             | 2.6370 | 0.3224| H-1→L (81%), H→L (16%)                               |
| 3   | 435.978             | 2.8438 | 0.8646| H→L+1 (85%), H→L+1 (5%), H→L+2 (4%)                  |
| 4   | 375.889             | 3.2984 | 0.1911| H-5→L (13%), H-1→L+1 (62%), H→L+1 (5%), H-3→L (8%),  |
\[ H \rightarrow L+1 \ (4\%) \]

| NO. | DFT \( \lambda \) (nm) | E (eV) | \( f \) | MO contributions |
|-----|-----------------|-------|-----|-----------------|
| 1   | 664.505         | 1.8658| 0.4558| \( H-1 \rightarrow L \ (11\%) \), \( H \rightarrow L \ (87\%) \) |
| 2   | 569.070         | 2.1787| 0.5143| \( H-1 \rightarrow L \ (82\%) \), \( H \rightarrow L \ (12\%) \) |
| 3   | 494.450         | 2.5075| 0.2124| \( H-1 \rightarrow L+1 \ (10\%) \), \( H \rightarrow L+1 \ (83\%) \), \( H \rightarrow L+2 \ (3\%) \) |
| 4   | 445.855         | 2.7808| 1.0276| \( H-4 \rightarrow L \ (14\%) \), \( H \rightarrow L+2 \ (51\%) \), \( H-5 \rightarrow L \ (9\%) \), \( H-3 \rightarrow L \ (8\%) \), \( H-1 \rightarrow L+2 \ (6\%) \), \( H \rightarrow L+1 \ (2\%) \), \( H \rightarrow L+3 \ (2\%) \) |
| 5   | 440.626         | 2.8138| 0.106 | \( H-1 \rightarrow L+1 \ (78\%) \), \( H \rightarrow L+1 \ (11\%) \), \( H-4 \rightarrow L+1 \ (2\%) \), \( H-3 \rightarrow L+1 \ (2\%) \) |
| 6   | 435.755         | 2.8518| 0.1345| \( H-4 \rightarrow L \ (19\%) \), \( H-3 \rightarrow L \ (28\%) \), \( H \rightarrow L+2 \ (30\%) \), \( H-5 \rightarrow L \ (4\%) \), \( H-2 \rightarrow L \ (8\%) \), \( H \rightarrow L+1 \ (2\%) \) |

\( MO= \)molecular orbital, \( H= \)HOMO, \( L= \)LUMO, \( f= \)oscillator strength.

**Table S16:** Wave length, excitation energy and oscillator strength of investigated compound (MCPTD2)

\[ MO= \)molecular orbital, \( H= \)HOMO, \( L= \)LUMO, \( f= \)oscillator strength.

| NO. | DFT \( \lambda \) (nm) | E (eV) | \( f \) | MO contributions |
|-----|-----------------|-------|-----|-----------------|
| 1   | 697.123         | 1.7785| 0.4535| \( H \rightarrow L \ (90\%) \), \( H-1 \rightarrow L \ (8\%) \) |
| 2   | 578.658         | 2.1426| 0.5421| \( H-1 \rightarrow L \ (84\%) \), \( H \rightarrow L \ (9\%) \) |
| 3   | 517.827         | 2.3943| 0.1583| \( H \rightarrow L+1 \ (86\%) \), \( H-1 \rightarrow L+1 \ (8\%) \) |
| 4   | 453.122         | 2.7362| 0.9009| \( H-4 \rightarrow L \ (13\%) \), \( H \rightarrow L+2 \ (46\%) \), \( H-5 \rightarrow L \ (9\%) \), \( H-3 \rightarrow L \ (8\%) \) |
| 5   | 451.736         | 2.7446| 0.3275| \( H-1 \rightarrow L+1 \ (72\%) \), \( H \rightarrow L+1 \ (11\%) \), \( H-4 \rightarrow L+1 \ (2\%) \) |
| 6   | 441.882         | 2.8058| 0.1248| \( H-4 \rightarrow L \ (15\%) \), \( H-3 \rightarrow L \ (31\%) \), \( H-2 \rightarrow L \ (10\%) \), \( H \rightarrow L+2 \ (33\%) \) |

\( MO= \)molecular orbital, \( H= \)HOMO, \( L= \)LUMO, \( f= \)oscillator strength.

**Table S17:** Wave length, excitation energy and oscillator strength of investigated compound (MCPTD3)
Table S18: Wave length, excitation energy and oscillator strength of investigated compound
(MCPTD4)

| NO. | DFT λ (nm) | E (eV)  | f    | MO contributions                                      |
|-----|------------|---------|------|-------------------------------------------------------|
| 1   | 720.205    | 1.7215  | 0.4299| H → L (91%), H-1 → L (8%)                             |
| 2   | 593.108    | 2.0904  | 0.5408| H-1 → L (86%), H → L (9%)                             |
| 3   | 529.052    | 2.3435  | 0.1662| H → L+1 (87%), H-1 → L+1 (8%)                         |
| 4   | 459.266    | 2.6996  | 0.2444| H-1 → L+1 (77%), H → L+1 (10%), H-4 → L+1 (2%), H-3 → L+1 (2%) |
| 5   | 457.132    | 2.7122  | 0.8075| H-5 → L (13%), H-4 (20%), H-3 → L (20%), H → L+2 (27%), H-2 → L (5%), H-1 → L+1 (6%), H-1 → L+2 (3%) |
| 6   | 446.529    | 2.7766  | 0.3056| H-3 → L (23%), H-2 → L (11%), H → L+2 (53%), H-4 → L (5%), H → L+3 (2%) |

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength.

Table S19: Wave length, excitation energy and oscillator strength of investigated compound
(MCPTD5)

| NO. | DFT λ (nm) | E (eV)  | f    | MO contributions                                      |
|-----|------------|---------|------|-------------------------------------------------------|
| 1   | 724.286    | 1.7118  | 0.4375| H → L (91%), H-1 → L (8%)                             |
| 2   | 596.246    | 2.0794  | 0.5567| H-1 → L (85%), H → L (9%)                             |
| 3   | 539.011    | 2.3002  | 0.1093| H → L+1 (88%), H-1 → L (2%), H-1 → L+1 (8%)           |
| 4   | 467.368    | 2.6528  | 0.1173| H-1 → L+1 (82%), H → L+1 (10%), H-4 → L+1 (2%), H-3 → L+1 (2%) |
| 5   | 459.283    | 2.6995  | 1.0156| H-5 → L (12%), H-4 → L (18%), H-3 → L (18%), H → L+2 (34%), H-1 → L (3%), H-1 → L+2 (4%) |
| 6   | 448.840    | 2.7623  | 0.2484| H-3 → L (25%), H-2 → L (13%), H-4 → L (7%)            |

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength.

Table 20: Wave length, excitation energy and oscillator strength of investigated compound
(MCPTD6)

| NO. | DFT λ (nm) | E (eV)  | f    | MO contributions                                      |
|-----|------------|---------|------|-------------------------------------------------------|
| 1   | 743.667    | 1.6672  | 0.3876| H-1 → L (92%),                                      |
| 2   | 609.738    | 2.0334  | 0.5522| H-1 → L (86%), H → L (8%)                             |
| 3   | 554.739    | 2.2350  | 0.0937| H → L+1 (88%), H-1 → L (2%), H-1 → L+1 (8%)            |

MO=molecular orbital, H=HOMO, L=LUMO, f= oscillator strength.
| NO. | DFT λ (nm) | E (eV) | F   | MO contributions |
|-----|------------|--------|-----|------------------|
| 4   | 479.592    | 2.5852 | 0.1313 | H-1→L+1 (83%), H-4→L+1 (2%), H-3→L+1 (2%), H→L+1 (9%) |
| 5   | 464.482    | 2.6693 | 0.7603 | H-5→L (14%), H-4→L (21%), H-3→L (30%), H→L+2 (14%), H-1→L (3%), H-1→L+2 (3%) |
| 6   | 452.348    | 2.7409 | 0.4850 | H-3→L (15%), H-2→L (16%), H→L+2 (59%), H-1→L+2 (2%) |

MO=molecular orbital, H=HOMO, L=LUMO, f=oscillator strength

**Table 21:** Wave length, excitation energy and oscillator strength of investigated Compound (MCPTD7)

| NO. | DFT λ (nm) | E (eV) | F   | MO contributions |
|-----|------------|--------|-----|------------------|
| 1   | 832.33     | 1.4896 | 0.2774 | H→L (94%), H-1→L (4%) |
| 2   | 669.85     | 1.8509 | 0.4875 | H-1→L (22%), H→L+1 (66%), H-1→L+1 (7%), H→L (3%) |
| 3   | 653.85     | 1.8962 | 0.1131 | H-1→L (69%), H→L+1 (26%), H→L (2%) |
| 4   | 552.51     | 2.2440 | 0.2039 | H-1→L+1 (87%), H→L+1 (7%) |
| 5   | 491.33     | 2.5234 | 0.286  | H-4→L (14%), H-3→L (44%), H-2→L (26%), H-5→L (8%), H-1→L (3%) |
| 6   | 477.96     | 2.5940 | 0.1161 | H-3→L (15%), H-2→L (73%), H-5→L (4%), H-4→L (4%), H→L+2 (2%) |

MO=molecular orbital, H=HOMO, L=LUMO, f=oscillator strength.

**Table S22:** Wave length, excitation energy and oscillator strength of investigated Compound (MCPTD8)

| NO. | DFT λ (nm) | E (eV) | F   | MO contributions |
|-----|------------|--------|-----|------------------|
| 1   | 691.60     | 1.7927 | 0.4879 | H-1→L (10%), H→L (89%) |
| 2   | 581.04     | 2.1338 | 0.5772 | H-1→L (84%), H→L (11%) |
| 3   | 475.58     | 2.6070 | 0.4446 | H→L+1 (74%), H→L+2 (12%), H-1→L+1 (7%) |
| 4   | 452.44     | 2.7403 | 0.5511 | H-4→L (40%), H-3→L (25%), H→L+1 (10%), H-5→L (5%), H-2→L (3%), H→L (2%), H-1→L+2 (3%), H→L+2 (9%) |
| 5   | 444.13     | 2.7916 | 0.3673 | H-6→L (11%), H→L+2 (54%), H-5→L (7%), H-4→L (8%), H-3→L (4%), H-1→L+1 (3%), H-1→L+2 (3%), H→L+1 (4%) |
| 6   | 434.91     | 2.8508 | 0.1283 | H-6→L (27%), H-5→L (26%), H-3→L (20%), H-4→L (3%), H-2→L (9%), H→L+1 (2%), H→L+2 (8%) |
| Donor(i) | Type | Acceptor(j) | Type | \( E \ (2)^a \) \([\text{kcal/mol}]\) | \( E(J)E(i)^b \) (a.u) | \( F(I\rightarrow j)^e \) (a.u) |
|---------|------|-------------|------|-----------------|-----------------|-----------------|
| C26-C28 | \( \pi \) | C31-O32 | \( \pi^* \) | 24.36 | 0.31 | 0.079 |
| C3-C4   | \( \pi \) | C8-C15 | \( \pi^* \) | 22.41 | 0.29 | 0.072 |
| C5-C6   | \( \pi \) | C1-C2 | \( \pi^* \) | 20.91 | 0.3 | 0.072 |
| C5-C6   | \( \pi \) | C3-C4 | \( \pi^* \) | 18.37 | 0.29 | 0.067 |
| C9-C11  | \( \pi \) | C7-C10 | \( \pi^* \) | 17.66 | 0.3 | 0.069 |
| C53-C54 | \( \pi \) | C56-C58 | \( \pi^* \) | 15.98 | 0.3 | 0.063 |
| C3-C4   | \( \pi \) | C7-C10 | \( \pi^* \) | 13.88 | 0.3 | 0.062 |
| C26-C28 | \( \pi \) | C53-C54 | \( \pi^* \) | 9.95 | 0.31 | 0.052 |
| C31-O32 | \( \pi \) | C31-O32 | \( \pi^* \) | 7.5 | 0.42 | 0.017 |
| O32     | LP(2) | C31-O33 | \( \sigma^* \) | 35.28 | 0.66 | 0.138 |
| S55     | LP(2) | C56-C58 | \( \pi^* \) | 25.1 | 0.28 | 0.075 |
| S55     | LP(2) | C53-C54 | \( \pi^* \) | 22.52 | 0.27 | 0.07 |
| O32     | LP(2) | C28-C31 | \( \sigma^* \) | 20.86 | 0.73 | 0.112 |
| N30     | LP(1) | C28-C29 | \( \sigma^* \) | 12.75 | 1.07 | 0.105 |
| O33     | LP(1) | C31-O32 | \( \sigma^* \) | 8.19 | 1.19 | 0.088 |
| O33     | LP(2) | C34-H36 | \( \sigma^* \) | 4.75 | 0.76 | 0.056 |
| O33     | LP(2) | C34-H37 | \( \sigma^* \) | 4.55 | 0.76 | 0.055 |
| O32     | LP(1) | C28-C31 | \( \sigma^* \) | 2.6 | 1.16 | 0.05 |
| S55     | LP(1) | C56-C58 | \( \sigma^* \) | 2.3 | 1.25 | 0.048 |
| S55     | LP(1) | C53-C54 | \( \sigma^* \) | 2.09 | 1.24 | 0.046 |
| S55     | LP(2) | C17-H18 | \( \sigma^* \) | 1.48 | 0.71 | 0.032 |
| O32     | LP(1) | C31-O33 | \( \sigma^* \) | 1.41 | 1.1 | 0.036 |
| O33     | LP(1) | C34-C35 | \( \sigma^* \) | 1.01 | 1.01 | 0.03 |
| O33     | LP(1) | C34-H37 | \( \sigma^* \) | 1.02 | 1.01 | 0.029 |
| O33     | LP(1) | C34-H36 | \( \sigma^* \) | 1.0 | 1.01 | 0.028 |
| O33     | LP(1) | C26-H27 | \( \sigma^* \) | 0.96 | 1.01 | 0.028 |
| O32     | LP(2) | C29-N30 | \( \pi^* \) | 0.87 | 0.39 | 0.017 |
| O32     | LP(2) | C34-C35 | \( \sigma^* \) | 0.8 | 0.7 | 0.022 |
| O33     | LP(1) | C28-C31 | \( \sigma^* \) | 0.68 | 1.03 | 0.024 |
| O33     | LP(1) | C35-C38 | \( \sigma^* \) | 0.61 | 1.01 | 0.022 |
| C26-H27 | \( \sigma \) | C28-C29 | \( \sigma^* \) | 6.92 | 1.07 | 0.077 |
| C29-N30 | \( \sigma \) | C28-C29 | \( \sigma^* \) | 5.99 | 1.58 | 0.088 |
| C28-C29 | \( \sigma \) | C29-N30 | \( \sigma^* \) | 5.47 | 1.6 | 0.084 |
| C17-H18 | \( \sigma \) | C4-C5 | \( \sigma^* \) | 4.0 | 1.09 | 0.059 |
| C38-H42 | \( \sigma \) | C43-H46 | \( \sigma^* \) | 3.0 | 0.92 | 0.047 |
| C8-C15  | \( \sigma \) | C14-H25 | \( \sigma^* \) | 2.04 | 1.13 | 0.043 |
| C56-H59 | \( \sigma \) | C56-C58 | \( \sigma^* \) | 1.96 | 1.11 | 0.042 |
| C1-C6   | \( \sigma \) | C1-H21 | \( \sigma^* \) | 1.0 | 1.15 | 0.03 |
| C34-C35 | \( \sigma \) | C35-H40 | \( \sigma^* \) | 0.51 | 1.06 | 0.021 |
| C34-H36 | \( \sigma \) | C34-C35 | \( \sigma^* \) | 0.51 | 0.94 | 0.019 |
| C35-H39 | \( \sigma \) | C35-C38 | \( \sigma^* \) | 0.51 | 0.91 | 0.019 |
| Donor(i)  | Type | Acceptor(j) | Type | $E(2)$ | $E(J)E(i)b$(a.u) | $F(I→j)e$(a.u) |
|----------|------|-------------|------|--------|------------------|----------------|
| C2-C3    | $\pi$ | C1-C6       | $\pi^*$ | 25.17  | 0.28             | 0.076          |
| C25-C27  | $\pi$ | C30-O31     | $\pi^*$ | 24.34  | 0.31             | 0.079          |
| C11-C12  | $\pi$ | C13-C14     | $\pi^*$ | 22.04  | 0.3              | 0.073          |
| C8-C9    | $\pi$ | C4-C5       | $\pi^*$ | 21.99  | 0.28             | 0.07           |
| C77-C79  | $\pi$ | C78-C80     | $\pi^*$ | 20.00  | 0.3              | 0.069          |
| C69-C73  | $\pi$ | C68-C71     | $\pi^*$ | 19.25  | 0.3              | 0.069          |
| C15-C16  | $\pi$ | C13-C14     | $\pi^*$ | 16.44  | 0.31             | 0.067          |
| C7-C10   | $\pi$ | C8-C9       | $\pi^*$ | 14.41  | 0.31             | 0.063          |
| C94-C110 | $\pi$ | C91-C93     | $\pi^*$ | 13.72  | 0.3              | 0.058          |
| C25-C27  | $\pi$ | C52-C53     | $\pi^*$ | 9.99   | 0.31             | 0.052          |
| C28-N29  | $\pi$ | C25-C27     | $\pi^*$ | 7.14   | 0.38             | 0.049          |
| C55-C57  | $\pi$ | C1-C6       | $\pi^*$ | 6.48   | 0.32             | 0.042          |
| C30-O31  | $\pi$ | C25-C27     | $\pi^*$ | 3.98   | 0.43             | 0.039          |
| C25-C27  | $\pi$ | C25-C27     | $\pi^*$ | 2.21   | 0.32             | 0.024          |
| C55-C57  | $\pi$ | C55-C57     | $\pi^*$ | 0.66   | 0.3              | 0.013          |
| O31      | LP(2) | C30-O32     | $\sigma^*$ | 35.26 | 0.66             | 0.138          |
| N76      | LP(1) | C69-C73     | $\pi^*$ | 24.99  | 0.29             | 0.079          |
| S54      | LP(2) | C55-C57     | $\pi^*$ | 24.97  | 0.28             | 0.075          |
| S61      | LP(2) | C62-C64     | $\pi^*$ | 23.61  | 0.29             | 0.074          |
| S54      | LP(2) | C52-C53     | $\pi^*$ | 22.58  | 0.27             | 0.07           |
| S61      | LP(2) | C59-C60     | $\pi^*$ | 22.50  | 0.29             | 0.072          |
| O31      | LP(2) | C27-C30     | $\sigma^*$ | 20.85 | 0.73             | 0.112          |
| N76      | LP(1) | C85-C86     | $\pi^*$ | 19.69  | 0.29             | 0.07           |
| N76      | LP(1) | C77-C79     | $\pi^*$ | 17.41  | 0.29             | 0.066          |
| N29      | LP(1) | C27-C28     | $\sigma^*$ | 12.76 | 1.07             | 0.105          |
| O32      | LP(1) | C30-O31     | $\sigma^*$ | 8.18  | 1.19             | 0.088          |
| O32      | LP(2) | C33-H35     | $\sigma^*$ | 4.78  | 0.76             | 0.056          |
| O32      | LP(2) | C33-H36     | $\sigma^*$ | 4.52  | 0.76             | 0.055          |
| N76      | LP(1) | C77-C78     | $\sigma^*$ | 3.53  | 0.84             | 0.052          |
| N76      | LP(1) | C77-C79     | $\sigma^*$ | 3.51  | 0.84             | 0.052          |
| N76      | LP(1) | C85-C87     | $\sigma^*$ | 3.17  | 0.84             | 0.049          |
| N76      | LP(1) | C85-C86     | $\sigma^*$ | 3.01  | 0.84             | 0.049          |
| O31      | LP(1) | C27-C30     | $\sigma^*$ | 2.60  | 1.16             | 0.05           |
| N76      | LP(1) | C71-C73     | $\sigma^*$ | 2.60  | 0.84             | 0.044          |
| N76      | LP(1) | C69-C73     | $\sigma^*$ | 2.57  | 0.84             | 0.044          |
| S54      | LP(1) | C55-C57     | $\sigma^*$ | 2.31  | 1.25             | 0.048          |
| S61      | LP(1) | C59-C60     | $\sigma^*$ | 2.12  | 1.25             | 0.046          |
| S61      | LP(1) | C62-C64     | $\sigma^*$ | 2.12  | 1.26             | 0.046          |
| S54      | LP(1) | C52-C53     | $\sigma^*$ | 2.09  | 1.24             | 0.046          |
| O31      | LP(1) | C30-O32     | $\sigma^*$ | 1.40  | 1.1              | 0.036          |
| S54      | LP(2) | C16-H17     | $\sigma^*$ | 1.37  | 0.71             | 0.031          |
Table S25: Natural bond orbital (NBO) analysis of (MCPTD2)

| Donor(i) | Type | Acceptor(j) | Type | E(2)   | E(J)E(i)b(a.u) | F(I→j)e(a.u) |
|---------|------|-------------|------|--------|----------------|---------------|
| C104-C110 | π     | C111-N112   | π*   | 23.02  | 0.4            | 0.088         |
| C47-C59   | π     | C41-C43     | π*   | 22.98  | 0.28           | 0.071         |
| C96-C101  | π     | C102-O109   | π*   | 20.01  | 0.29           | 0.071         |
| C49-C50   | π     | C51-C53     | π*   | 19.97  | 0.3            | 0.069         |
| C37-C126  | π     | C34-C35     | π*   | 17.70  | 0.31           | 0.069         |
| C34-C35   | π     | C37-C126    | π*   | 16.33  | 0.31           | 0.066         |
| C116-C117 | π     | C37-C126    | π*   | 15.58  | 0.28           | 0.06          |
| C25-C103  | π     | C27-C28     | π*   | 10.75  | 0.29           | 0.052         |
| C11-C12   | π     | C34-C35     | π*   | 9.89   | 0.29           | 0.048         |
| C102-O109 | π     | C96-C101    | π*   | 4.04   | 0.43           | 0.041         |
| C102-O109 | π     | C25-C103    | π*   | 3.70   | 0.43           | 0.038         |
| C113-N114 | π     | C111-N112   | π*   | 0.70   | 0.46           | 0.016         |
| N40       | LP(1) | C119-C123   | π*   | 25.12  | 0.29           | 0.079         |
| S36       | LP(2) | C37-C126    | π*   | 23.71  | 0.29           | 0.074         |
| S36       | LP(2) | C34-C35     | π*   | 22.56  | 0.29           | 0.072         |
| S29       | LP(2) | C27-C28     | π*   | 22.5   | 0.27           | 0.069         |
| O109      | LP(2) | C96-C102    | σ*   | 21.82  | 0.76           | 0.117         |
| O109      | LP(2) | C102-C103   | σ*   | 19.45  | 0.76           | 0.11          |
| N40       | LP(1) | C49-C50     | π*   | 18.42  | 0.29           | 0.068         |
| N40       | LP(1) | C41-C43     | π*   | 17.99  | 0.29           | 0.067         |
| N112      | LP(1) | C110-C111   | σ*   | 13.41  | 1.06           | 0.107         |
| N114      | LP(1) | C110-C113   | σ*   | 13.41  | 1.06           | 0.107         |
| O109      | LP(1) | C102-C103   | σ*   | 3.60   | 1.18           | 0.059         |
| N40       | LP(1) | C41-C42     | σ*   | 3.55   | 0.84           | 0.052         |
| N40       | LP(1) | C49-C51     | σ*   | 3.49   | 0.84           | 0.051         |
| N40       | LP(1) | C41-C43     | σ*   | 3.28   | 0.84           | 0.05          |
| Donor(i)  | Type | Acceptor(j) | Type | E(2)  | E(J)E(i)b(a.u) | F(I→j)e(a.u) |
|-----------|------|-------------|------|-------|----------------|---------------|
| O109      | LP(2)| S29-C32     | σ*   | 3.22  | 0.51           | 0.037         |
| N40       | LP(1)| C49-C50     | σ*   | 3.19  | 0.84           | 0.049         |
| S29       | LP(1)| C30-C32     | σ*   | 2.60  | 1.24           | 0.051         |
| N40       | LP(1)| C119-C123   | σ*   | 2.58  | 0.84           | 0.044         |
| N40       | LP(1)| C121-C123   | σ*   | 2.55  | 0.84           | 0.044         |
| S36       | LP(1)| C37-C126    | σ*   | 2.12  | 1.26           | 0.046         |
| S36       | LP(1)| C34-C35     | σ*   | 2.11  | 1.25           | 0.046         |
| S29       | LP(1)| C27-C28     | σ*   | 1.85  | 1.23           | 0.043         |
| O109      | LP(1)| S29-C32     | σ*   | 1.79  | 0.93           | 0.037         |
| S29       | LP(2)| C16-H17     | σ*   | 1.52  | 0.71           | 0.032         |
| O109      | LP(1)| C96-C102    | σ*   | 1.30  | 1.19           | 0.035         |
| C25-H26   | σ   | C102-C103   | σ*   | 6.78  | 1              | 0.074         |
| C96-C101  | σ   | C96-C97     | σ*   | 5.00  | 1.3            | 0.072         |
| C1-H20    | σ   | C2-C3       | σ*   | 4.00  | 1.11           | 0.06          |
| C116-C126 | σ   | C116-C118   | σ*   | 3.00  | 1.27           | 0.055         |
| N40-C49   | σ   | C119-C123   | σ*   | 2.00  | 1.35           | 0.046         |
| C98-C99   | σ   | C99-H106    | σ*   | 1.00  | 1.17           | 0.031         |

**Table S26: Natural bond orbital (NBO) analysis of (MCPTD3)**
| Donor(i) | Type | Acceptor(j) | Type | E(2)  | E(JE(i)b(a.u) | F(I→j)e(a.u) |
|---------|------|-------------|------|-------|---------------|--------------|
| C25-C103 | π    | C104-C107   | π*   | 26.74 | 0.3           | 0.08         |
| C13-C14  | π    | C11-C12     | π*   | 23.09 | 0.29          | 0.073        |
| C65-C67  | π    | C60-C64     | π*   | 21.00 | 0.3           | 0.072        |
| C4-C5    | π    | C1-C6       | π*   | 20.01 | 0.28          | 0.068        |
| C97-C98  | π    | C96-C101    | π*   | 19.80 | 0.29          | 0.069        |
| C7-C10   | π    | C2-C3       | π*   | 17.53 | 0.31          | 0.069        |
| C2-C3    | π    | C7-C10      | π*   | 16.99 | 0.31          | 0.068        |

TableS27: Natural bond orbital (NBO) analysis of (MCPTD4)
| Bond          | Bonding Type | Acceptable Bond Type | Bond Energy (kcal/mol) | Bond Length (Å) | Number of Bonds |
|---------------|--------------|----------------------|-----------------------|----------------|-----------------|
| C8-C9         | π            | C7-C10                | 15.14                 | 0.3            | 0.065           |
| C7-C10        | π            | C8-C9                 | 14.44                 | 0.31           | 0.063           |
| C25-C103      | π            | C27-C28               | 14.44                 | 0.29           | 0.052           |
| C11-C12       | π            | C34-C35               | 9.44                  | 0.29           | 0.047           |
| C108-N109     | π            | C104-C107             | 6.79                  | 0.38           | 0.049           |
| C102-O106     | π            | C96-C101              | 4.22                  | 0.41           | 0.041           |
| S29           | LP(2)        | C30-C32               | 26.83                 | 0.27           | 0.077           |
| S36           | LP(2)        | C37-C125              | 23.64                 | 0.29           | 0.073           |
| O106          | LP(2)        | C96-C102              | 23.56                 | 0.75           | 0.121           |
| F126          | LP(3)        | C96-C101              | 23                    | 0.46           | 0.1             |
| F113          | LP(3)        | C99-C100              | 22.47                 | 0.44           | 0.097           |
| S36           | LP(2)        | C34-C35               | 22.41                 | 0.29           | 0.072           |
| S29           | LP(2)        | C27-C28               | 22.27                 | 0.26           | 0.069           |
| F114          | LP(3)        | C99-C100              | 21.10                 | 0.44           | 0.094           |
| O106          | LP(2)        | C102-C103             | 19.08                 | 0.75           | 0.109           |
| N40           | LP(1)        | C49-C50               | 17.39                 | 0.29           | 0.066           |
| N40           | LP(1)        | C41-C43               | 14.92                 | 0.29           | 0.061           |
| N109          | LP(1)        | C107-C108             | 13.46                 | 1.06           | 0.107           |
| N111          | LP(1)        | C107-C110             | 13.45                 | 1.06           | 0.107           |
| F126          | LP(2)        | C100-C101             | 8.35                  | 0.98           | 0.081           |
| F113          | LP(2)        | C99-C100              | 8.34                  | 0.98           | 0.081           |
| F114          | LP(2)        | C99-C100              | 8.04                  | 0.98           | 0.079           |
| F114          | LP(2)        | C100-C101             | 8.03                  | 0.98           | 0.079           |
| F126          | LP(2)        | C96-C101              | 7.66                  | 1.02           | 0.079           |
| F113          | LP(2)        | C98-C99               | 6.7                   | 1.01           | 0.074           |
| N40           | LP(1)        | C41-C42               | 4.00                  | 0.84           | 0.055           |
| N40           | LP(1)        | C41-C43               | 3.84                  | 0.84           | 0.054           |
| O106          | LP(1)        | C102-C103             | 3.81                  | 1.18           | 0.06            |
| N40           | LP(1)        | C49-C51               | 3.63                  | 0.84           | 0.053           |
| N40           | LP(1)        | C49-C50               | 3.39                  | 0.84           | 0.051           |
| O106          | LP(2)        | C29-C32               | 3.35                  | 0.51           | 0.038           |
| S29           | LP(1)        | C30-C32               | 2.61                  | 1.24           | 0.051           |
| S36           | LP(1)        | C34-C35               | 2.12                  | 1.25           | 0.046           |
| S36           | LP(1)        | C37-C125              | 2.10                  | 1.26           | 0.046           |
| N40           | LP(1)        | C120-C122             | 2.02                  | 0.83           | 0.039           |
| N40           | LP(1)        | C118-C122             | 1.94                  | 0.84           | 0.038           |
| S29           | LP(1)        | C27-C28               | 1.85                  | 1.23           | 0.043           |
| O106          | LP(1)        | S29-C32               | 1.82                  | 0.94           | 0.037           |
| F126          | LP(1)        | C96-C101              | 1.73                  | 1.64           | 0.048           |
| F113          | LP(1)        | C98-C99               | 1.65                  | 1.63           | 0.046           |
| S29           | LP(2)        | C16-H17               | 1.59                  | 0.71           | 0.033           |
| F114          | LP(1)        | C99-C100              | 1.37                  | 1.6            | 0.042           |
| F114          | LP(1)        | C100-C101             | 1.37                  | 1.61           | 0.042           |
| Donor(i)   | Type | Acceptor(j) | Type | $E(2)$  | $E(J)E(i)b(a.u)$ | $F(I\to j)e(a.u)$ |
|------------|------|-------------|------|---------|-----------------|------------------|
| C25-C103  | $\pi$ | C104-C107   | $\pi^*$| 26.37   | 0.3             | 0.079            |
| C2-C3     | $\pi$ | C1-C6       | $\pi^*$| 25.7    | 0.28            | 0.077            |
| C62-C63   | $\pi$ | C65-C67     | $\pi^*$| 22.92   | 0.29            | 0.073            |
| C99-C100  | $\pi$ | C97-C98     | $\pi^*$| 19.23   | 0.33            | 0.071            |
| C96-C101  | $\pi$ | C102-O106   | $\pi^*$| 18.94   | 0.3             | 0.07             |
| C34-C35   | $\pi$ | C37-C123    | $\pi^*$| 16.28   | 0.31            | 0.066            |
| C15-C16   | $\pi$ | C4-C5       | $\pi^*$| 15.32   | 0.3             | 0.065            |
| C4-C5     | $\pi$ | C15-C16     | $\pi^*$| 14.42   | 0.3             | 0.063            |
| C57-C73   | $\pi$ | C54-C56     | $\pi^*$| 13.74   | 0.3             | 0.058            |
| C60-C64   | $\pi$ | C47-C59     | $\pi^*$| 13.70   | 0.3             | 0.058            |
| C1-C6     | $\pi$ | C30-C32     | $\pi^*$| 12.75   | 0.27            | 0.053            |
| C104-C107 | $\pi$ | C97-C98     | $\pi^*$| 9.05    | 0.32            | 0.05             |
| C104-C107 | $\pi$ | C25-C103    | $\pi^*$| 7.77    | 0.33            | 0.046            |
| C102-O106 | $\pi$ | C96-C101    | $\pi^*$| 4.16    | 0.43            | 0.041            |
| S29       | LP(2) | C30-C32     | $\pi^*$| 26.8    | 0.27            | 0.077            |
| S36       | LP(2) | C37-C123    | $\pi^*$| 23.64   | 0.29            | 0.073            |
| S36       | LP(2) | C34-C35     | $\pi^*$| 22.43   | 0.29            | 0.072            |
| O106      | LP(2) | C96-C102    | $\sigma^*$| 22.29 | 0.76            | 0.118            |
| S29       | LP(2) | C27-C28     | $\pi^*$| 22.28   | 0.27            | 0.069            |
| O106      | LP(2) | C102-C103   | $\sigma^*$| 19.38 | 0.76            | 0.11             |
| N40       | LP(1) | C49-C50     | $\pi^*$| 17.03   | 0.29            | 0.065            |
| C1125     | LP(3) | C99-C100    | $\pi^*$| 16.02   | 0.31            | 0.07             |
| C1126     | LP(3) | C99-C100    | $\pi^*$| 15.77   | 0.31            | 0.069            |
| N40       | LP(1) | C41-C43     | $\pi^*$| 15.26   | 0.29            | 0.061            |
| N109      | LP(1) | C107-C108   | $\sigma^*$| 13.45 | 1.06            | 0.107            |
| N111      | LP(1) | C107-C110   | $\sigma^*$| 13.44 | 1.06            | 0.107            |
| C1125     | LP(2) | C99-C100    | $\sigma^*$| 5.38  | 0.86            | 0.061            |
| C1126     | LP(2) | C99-C100    | $\sigma^*$| 5.25  | 0.86            | 0.06             |
| C1125     | LP(2) | C100-C101   | $\sigma^*$| 3.97  | 0.89            | 0.053            |
| N40       | LP(1) | C41-C42     | $\sigma^*$| 3.95  | 0.84            | 0.055            |
| Donor(i)    | Type       | Acceptor(j)       | Type  | E(2)  | E(J)E(i)b(a.u) | F(I→j)e(a.u) |
|------------|------------|-------------------|-------|-------|----------------|--------------|
| C25-C103   |            | C104-C107         |      | 27.31 | 0.29           | 0.08         |
| C97-C98    |            | C96-C101          |      | 23.00 | 0.28           | 0.073        |
| C65-C67    |            | C60-C64           |      | 21.00 | 0.3            | 0.072        |
| C4-C5      |            | C1-C6             |      | 20.00 | 0.28           | 0.068        |
| C99-C100   |            | C96-C101          |      | 18.31 | 0.32           | 0.069        |
| C99-C100   |            | C97-C98           |      | 18.25 | 0.33           | 0.07         |
| C37-C123   |            | C34-C35           |      | 17.83 | 0.31           | 0.069        |
| C102-O106  |            | C102-C103         |      | 1.69  | 1.57           | 0.047        |
| C30-C32    |            | C27-S29           |      | 0.52  | 0.93           | 0.02         |

Table S29: Natural bond orbital (NBO) analysis of (MCPTD6)
| Bond          | Type | Bond         | Type |  \( \delta \) |  \( \delta^* \) |  \( \sigma \) |  \( \sigma^* \) |
|---------------|------|--------------|------|--------------|---------------|-------------|---------------|
| C104-C107     | \( \pi \) | C25-C103     | \( \pi^* \) | 7.97         | 0.33          | 0.047       |
| C110-N111     | \( \pi \) | C108-N109    | \( \pi^* \) | 0.72         | 0.46          | 0.016       |
| S29           | LP(2) | C30-C32      | \( \pi^* \) | 26.90        | 0.27          | 0.077       |
| O106          | LP(2) | C96-C102     | \( \delta^* \) | 23.96        | 0.74          | 0.121       |
| S36           | LP(2) | C37-C123     | \( \pi^* \) | 23.65        | 0.29          | 0.074       |
| S36           | LP(2) | C34-C35      | \( \pi^* \) | 22.48        | 0.29          | 0.072       |
| S29           | LP(2) | C27-C28      | \( \pi^* \) | 22.22        | 0.26          | 0.069       |
| O106          | LP(2) | C102-C103    | \( \delta^* \) | 18.85        | 0.76          | 0.109       |
| N40           | LP(1) | C49-C50      | \( \pi^* \) | 17.21        | 0.29          | 0.065       |
| Cl124         | LP(3) | C99-C100     | \( \pi^* \) | 16.58        | 0.31          | 0.071       |
| Cl125         | LP(3) | C99-C100     | \( \pi^* \) | 16.33        | 0.31          | 0.07        |
| Cl126         | LP(3) | C96-C101     | \( \pi^* \) | 15.86        | 0.34          | 0.071       |
| N40           | LP(1) | C41-C43      | \( \pi^* \) | 15.19        | 0.29          | 0.061       |
| N109          | LP(1) | C107-C108    | \( \sigma^* \) | 13.50        | 1.06          | 0.107       |
| N111          | LP(1) | C107-C110    | \( \sigma^* \) | 13.47        | 1.06          | 0.107       |
| Cl125         | LP(2) | C99-C100     | \( \sigma^* \) | 5.47         | 0.86          | 0.061       |
| Cl126         | LP(2) | C100-C101    | \( \sigma^* \) | 5.18         | 0.85          | 0.059       |
| Cl124         | LP(2) | C100-C101    | \( \sigma^* \) | 5.11         | 0.85          | 0.059       |
| Cl124         | LP(2) | C99-C100     | \( \sigma^* \) | 5.02         | 0.86          | 0.059       |
| Cl126         | LP(2) | C96-C101     | \( \sigma^* \) | 4.75         | 0.9           | 0.059       |
| N40           | LP(1) | C41-C42      | \( \sigma^* \) | 3.95         | 0.84          | 0.055       |
| N40           | LP(1) | C41-C43      | \( \sigma^* \) | 3.80         | 0.84          | 0.054       |
| Cl125         | LP(2) | C98-C99      | \( \sigma^* \) | 3.73         | 0.89          | 0.052       |
| N40           | LP(1) | C49-C51      | \( \sigma^* \) | 3.66         | 0.84          | 0.053       |
| O106          | LP(1) | C102-C103    | \( \sigma^* \) | 3.63         | 1.18          | 0.059       |
| N40           | LP(1) | C49-C50      | \( \sigma^* \) | 3.42         | 0.84          | 0.051       |
| O106          | LP(2) | S29-C32      | \( \sigma^* \) | 3.23         | 0.51          | 0.037       |
| S29           | LP(1) | C30-C32      | \( \sigma^* \) | 2.60         | 1.24          | 0.051       |
| S36           | LP(1) | C34-C35      | \( \sigma^* \) | 2.13         | 1.25          | 0.046       |
| S36           | LP(1) | C37-C123     | \( \sigma^* \) | 2.11         | 1.26          | 0.046       |
| N40           | LP(1) | C118-C120    | \( \sigma^* \) | 2.04         | 0.83          | 0.039       |
| N40           | LP(1) | C116-C120    | \( \sigma^* \) | 1.96         | 0.84          | 0.039       |
| S29           | LP(1) | C27-C28      | \( \sigma^* \) | 1.85         | 1.23          | 0.043       |
| O106          | LP(1) | S29-C32      | \( \sigma^* \) | 1.82         | 0.94          | 0.037       |
| S29           | LP(2) | C16-H17      | \( \sigma^* \) | 1.70         | 0.71          | 0.034       |
| Cl126         | LP(1) | C96-C101     | \( \sigma^* \) | 1.56         | 1.52          | 0.044       |
| Cl124         | LP(1) | C99-C100     | \( \sigma^* \) | 1.48         | 1.48          | 0.042       |
| Cl125         | LP(1) | C98-C99      | \( \sigma^* \) | 1.47         | 1.51          | 0.042       |
| Cl124         | LP(1) | C100-C101    | \( \sigma^* \) | 1.46         | 1.47          | 0.042       |
| Cl126         | LP(1) | C100-C101    | \( \sigma^* \) | 1.41         | 1.47          | 0.041       |
| Cl125         | LP(1) | C99-C100     | \( \sigma^* \) | 1.27         | 1.47          | 0.039       |
| O106          | LP(1) | C96-C102     | \( \sigma^* \) | 1.24         | 1.16          | 0.034       |
| S29           | LP(1) | C16-H17      | \( \sigma^* \) | 0.75         | 1.13          | 0.026       |
| Donor(i)     | Type  | Acceptor(j) | Type  | E(2) | E(J)E(i)b(a.u) | F(I→j)e(a.u) |
|-------------|-------|-------------|-------|------|----------------|--------------|
| C25-C103    | π     | C104-C107   | π*    | 27.52| 0.29           | 0.08         |
| C54-C56     | π     | C49-C50     | π*    | 23.06| 0.28           | 0.072        |
| C62-C63     | π     | C65-C67     | π*    | 22.93| 0.29           | 0.073        |
| C65-C67     | π     | C60-C64     | π*    | 21.00| 0.3            | 0.072        |
| C49-C50     | π     | C51-C53     | π*    | 20.04| 0.3            | 0.069        |
| C8-C9       | π     | C13-C14     | π*    | 19.75| 0.29           | 0.068        |
| C96-C101    | π     | C102-O106   | π*    | 17.64| 0.3            | 0.068        |
| C27-C28     | π     | C30-C32     | π*    | 16.7 | 0.29           | 0.063        |
| C7-C10      | π     | C3-C4       | π*    | 15.97| 0.31           | 0.067        |
| C5-C6       | π     | C15-C16     | π*    | 15.34| 0.31           | 0.065        |
| C102-O106   | π     | C96-C101    | π*    | 4.25 | 0.42           | 0.041        |
| C102-O106   | π     | C25-C103    | π*    | 3.66 | 0.43           | 0.038        |
| C30-C32     | π     | C30-C32     | π*    | 1.12 | 0.29           | 0.016        |
| C49-C50     | π     | C41-C43     | π*    | 0.72 | 0.29           | 0.013        |
| C108-N109   | π     | C110-N111   | π*    | 0.70 | 0.46           | 0.016        |
| S36         | LP(2) | C37-C123    | π*    | 27.26| 0.29           | 0.074        |
| O106        | LP(2) | C96-C102    | σ*    | 23.68| 0.75           | 0.118        |
| S36         | LP(2) | C34-C35     | π*    | 22.80| 0.29           | 0.072        |
| S29         | LP(2) | C27-C28     | π*    | 22.41| 0.26           | 0.068        |
| O106        | LP(2) | C102-C103   | σ*    | 21.90| 0.76           | 0.11         |
| O106        | LP(2) | S29-C32     | σ*    | 19.20| 0.51           | 0.036        |
| S29         | LP(2) | C16-H17     | σ*    | 16.94| 0.71           | 0.034        |
| N40         | LP(1) | C116-C120   | π*    | 14.83| 0.29           | 0.085        |
| N40         | LP(1) | C49-C50     | π*    | 13.5 | 0.29           | 0.065        |
| N40         | LP(1) | C41-C43     | π*    | 13.48| 0.29           | 0.06         |
| N109        | LP(1) | C107-C108   | σ*    | 13.2 | 1.06           | 0.107        |
| N111        | LP(1) | C107-C110   | σ*    | 13.18| 1.06           | 0.107        |
| N128        | LP(1) | C99-C127    | σ*    | 4.00 | 1.06           | 0.106        |
| N126        | LP(1) | C100-C125   | σ*    | 3.85 | 1.07           | 0.106        |
| N40         | LP(1) | C41-C42     | σ*    | 3.69 | 0.84           | 0.055        |
| N40         | LP(1) | C41-C43     | σ*    | 3.67 | 0.84           | 0.054        |
| N40         | LP(1) | C49-C51     | σ*    | 3.45 | 0.84           | 0.053        |
| O106        | LP(1) | C102-C103   | σ*    | 3.11 | 1.19           | 0.06         |
| N40         | LP(1) | C49-C50     | σ*    | 2.59 | 0.84           | 0.051        |
| S29         | LP(1) | C30-C32     | σ*    | 2.12 | 1.23           | 0.051        |
| Donor(i)       | Type | Acceptor(j)     | Type | E(2)  | E(J)E(i)b(a.u) | F(I→j)e(a.u) |
|---------------|------|-----------------|------|-------|----------------|--------------|
| C25-C103      | π    | C104-C107       | π*   | 25.87 | 0.3            | 0.079        |
| C116-C120     | π    | C113-C114       | π*   | 24.29 | 0.30           | 0.077        |
| C71-C72       | π    | C74-C76         | π*   | 22.29 | 0.29           | 0.073        |
| C49-C50       | π    | C54-C56         | π*   | 22.50 | 0.31           | 0.076        |
| C115-C118     | π    | C116-C120       | π*   | 21.37 | 0.29           | 0.073        |
| C62-C63       | π    | C60-C64         | π*   | 21.01 | 0.3            | 0.072        |
| C51-C53       | π    | C54-C56         | π*   | 20.99 | 0.31           | 0.073        |
| C97-C98       | π    | C104-C107       | π*   | 20.16 | 0.29           | 0.068        |
| C2-C3         | π    | C4-C5           | π*   | 19.60 | 0.29           | 0.068        |
| C96-C101      | π    | C97-C98         | π*   | 19.91 | 0.31           | 0.067        |
| C8-C9         | π    | C7-C10          | π*   | 15.05 | 0.3            | 0.064        |
| C7-C10        | π    | C8-C9           | π*   | 14.47 | 0.31           | 0.064        |
| C60-C64       | π    | C47-C59         | π*   | 13.69 | 0.3            | 0.058        |
| C127-C129     | π    | C90-C100        | π*   | 18.35 | 0.29           | 0.069        |
| C113-C114     | π    | C37-C123        | π*   | 15.88 | 0.28           | 0.060        |
| C99-C100      | π    | C96-C101        | π*   | 17.47 | 0.29           | 0.068        |
| C99-C100      | π    | C97-C98         | π*   | 18.22 | 0.29           | 0.068        |
| C99-C100      | π    | C125-C131       | π*   | 16.27 | 0.29           | 0.066        |
| C97-C98       | π    | C96-C101        | π*   | 17.72 | 0.32           | 0.068        |
| C97-C98       | π    | C99-C100        | π*   | 16.43 | 0.30           | 0.066        |
| S29           | LP(2) | C27-C28        | π*   | 22.47 | 0.27           | 0.069        |
| S36           | LP(2) | C34-C35        | π*   | 22.55 | 0.29           | 0.72         |
| S36           | LP(2) | C37-C123       | π*   | 23.61 | 0.29           | 0.73         |
| N40           | LP(1) | C41-C43        | π*   | 15.85 | 0.29           | 0.063        |
| N40           | LP(1) | C49-C50        | π*   | 3.08  | 0.84           | 0.049        |
| N40           | LP(1) | C49-C50        | π*   | 19.20 | 0.29           | 0.069        |
| O106          | LP(2) | C96-C102       | σ*   | 21.67 | 0.77           | 0.117        |
| O106          | LP(2) | C102-C103       | σ*   | 19.44 | 0.75           | 0.110        |

Table S31: Natural bond orbital (NBO) analysis of (MCPTD8)
|   |      |      |       |       |       |
|---|------|------|-------|-------|-------|
| N109 | LP(1) | C107-C108 | $\sigma^*$ | 13.38 | 1.07  | 0.107 |
| N111 | LP(1) | C107-C110  | $\sigma^*$ | 13.40 | 1.07  | 0.107 |
| O106 | LP(1) | C102-C103  | $\sigma^*$ |  3.61 | 1.18  | 0.059 |
| N40  | LP(1) | C41-C42    | $\sigma^*$ |  3.87 | 0.84  | 0.054 |
| C50-C56 | $\sigma$ | C54-C56  | $\sigma^*$ |  4.99 | 1.3   | 0.072 |
| C2-H21 | $\sigma$ | C1-C6    | $\sigma^*$ |  4.20 | 1.09  | 0.060 |
| C2-H21 | $\sigma$ | C3-C4    | $\sigma^*$ |  4.71 | 1.09  | 0.064 |
| C25-C103 | $\sigma$ | C25-C27  | $\sigma^*$ |  4.37 | 1.30  | 0.067 |
| C27-C28 | $\sigma$ | C25-C27  | $\sigma^*$ |  4.18 | 1.27  | 0.065 |
| C57-C71 | $\sigma$ | C50-C56  | $\sigma^*$ |  4.10 | 1.29  | 0.065 |
| C57-C71 | $\sigma$ | C57-C73  | $\sigma^*$ |  4.36 | 1.28  | 0.067 |
| C7-H19 | $\sigma$ | C9-C10   | $\sigma^*$ |  4.76 | 1.07  | 0.064 |
| C8-C14 | $\sigma$ | C8-C9    | $\sigma^*$ |  3.63 | 1.25  | 0.060 |
| C10-H22 | $\sigma$ | C3-C7    | $\sigma^*$ |  4.67 | 1.08  | 0.063 |
| C15-C18 | $\sigma$ | C8-C14   | $\sigma^*$ |  4.33 | 1.10  | 0.062 |
| C15-C18 | $\sigma$ | C5-C16   | $\sigma^*$ |  4.89 | 1.07  | 0.064 |
| C57-C73 | $\sigma$ | C54-C56  | $\sigma^*$ |  4.08 | 1.24  | 0.063 |
| C56-C57 | $\sigma$ | C50-C56  | $\sigma^*$ |  3.69 | 1.26  | 0.061 |
| C57-C71 | $\sigma$ | C50-C56  | $\sigma^*$ |  4.10 | 1.29  | 0.065 |
| C42-C44 | $\sigma$ | N40-C41  | $\sigma^*$ |  4.09 | 1.13  | 0.061 |
| C127-H128 | $\sigma$ | C129-C131 | $\sigma^*$ |  4.00 | 1.09  | 0.059 |
| C99-C100 | $\sigma$ | C100-C101 | $\sigma^*$ |  3.00 | 1.25  | 0.055 |
| N40-C49 | $\sigma$ | C116-C120 | $\sigma^*$ |  2.01 | 1.35  | 0.047 |
| N40-C41 | $\sigma$ | N40-C49  | $\sigma^*$ |  1.98 | 1.2   | 0.044 |
| C1-C6  | $\sigma$ | C1-H20   | $\sigma^*$ |  1.00 | 1.15  | 0.03  |

$^a$ E (2) means energy of hyper conjugative interaction (stabilization energy).

$^b$ Energy difference between donor and acceptor i and j NBO orbitals.

$^c$ $F(i\rightarrow j)$ is the Fock matrix element between i and j NBO orbitals.
Figure S1: Pictographic display of HOMO and LUMO of MCPTR-MCPTD8

Figure S2: Graph of investigated compound MCPTR
Figure S3: Graph of investigated compound MCPTD1

Figure S4: Graph of investigated compound MCPTD2
Figure S5: Graph of investigated compound MCPTD3

Figure S6: Graph of investigated compound MCPTD4
Figure S7: Graph of investigated compound MCPTD5

Figure S8: Graph of investigated compound MCPTD6
Figure S9: Graph of investigated compound MCPTD7

Figure S10: Graph of investigated compound MCPTD8