**Supplementary Data**

# Unveiling the Influence of End-capped Acceptors Modification on Photovoltaic Properties of Non-Fullerene Fused Ring Compounds: A DFT/TD-DFT Study

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**Table S1**: Cartesian coordinates of **NBR** compound.

| Atoms | X-axis | Y-axis | Z-axis |
|---|---|---|---|
| C | -2.142938 | -2.010308 | -0.132199 |
| C | -0.808943 | -2.302666 | -0.144345 |
| C | 0.157038 | -1.256349 | -0.051983 |
| C | -0.284834 | 0.111447 | 0.054128 |
| C | -1.67033 | 0.390788 | 0.065366 |
| H | 1.875854 | -2.56476 | -0.14226 |
| H | -0.456989 | -3.326136 | -0.223936 |
| C | 1.542381 | -1.535974 | -0.062289 |
| C | 0.681328 | 1.157796 | 0.14607 |
| H | -2.003207 | 1.419723 | 0.146089 |
| C | 2.448591 | -0.498736 | 0.028991 |
| H | 0.329471 | 2.181282 | 0.22545 |
| C | 2.015552 | 0.866009 | 0.134198 |
| C | 3.213744 | 1.818609 | 0.221585 |
| C | 4.367337 | 0.824783 | 0.153653 |
| C | -2.577861 | -0.646021 | -0.025777 |
| C | -4.490666 | -1.966643 | -0.150815 |
| C | -3.340517 | -2.963559 | -0.219656 |
| C | -4.021875 | -0.662109 | -0.03973 |

| | | | |
|---|---|---|---|
| C | -5.877731 | -2.087637 | -0.173288 |
| C | -6.598491 | -0.885998 | -0.080699 |
| H | -6.401741 | -3.033043 | -0.256028 |
| C | 3.890973 | -0.477776 | 0.045054 |
| C | 5.756169 | 0.968219 | 0.178043 |
| C | 6.473639 | -0.227535 | 0.086977 |
| H | 6.279658 | 1.909802 | 0.256427 |
| C | 7.853174 | -0.544332 | 0.086994 |
| C | 9.003157 | 0.223538 | 0.093095 |
| C | 9.109599 | 1.703342 | -0.019275 |
| C | 10.364927 | -0.314467 | 0.097225 |
| C | 10.546552 | 2.008092 | -0.186035 |
| C | 11.293243 | 0.821421 | -0.138376 |
| H | 8.029096 | -1.612023 | 0.058062 |
| C | 12.678769 | 0.875957 | -0.293136 |
| C | 13.246282 | 2.129827 | -0.48628 |
| C | 12.51685 | 3.314552 | -0.527288 |
| C | 11.135499 | 3.250341 | -0.37316 |
| H | 13.324342 | 0.011877 | -0.276949 |
| H | 13.034759 | 4.252784 | -0.679208 |
| H | 10.525766 | 4.145008 | -0.399417 |
| C | 10.772657 | -1.613999 | 0.334146 |
| C | 9.900346 | -2.687379 | 0.677313 |
| N | 9.242896 | -3.593748 | 0.969836 |
| C | 12.135438 | -2.028339 | 0.297607 |
| N | 13.224254 | -2.418901 | 0.276737 |
| C | 3.220922 | 2.599146 | 1.553748 |
| H | 3.197276 | 1.920089 | 2.408799 |
| H | 4.119939 | 3.216257 | 1.628111 |
| H | 2.351433 | 3.258574 | 1.613349 |
| C | 3.247271 | 2.797847 | -0.972134 |
| H | 2.38166 | 3.464475 | -0.943917 |
| H | 4.149617 | 3.413414 | -0.933979 |
| H | 3.236892 | 2.260488 | -1.922873 |
| C | -3.3722 | -3.943288 | 0.973681 |
| H | -4.272627 | -4.561873 | 0.935456 |
| H | -2.505148 | -4.608088 | 0.945904 |
| H | -3.363568 | -3.406213 | 1.924592 |
| C | -3.346753 | -3.743914 | -1.551892 |
| H | -3.324238 | -3.064637 | -2.406812 |
| H | -2.476537 | -4.402357 | -1.612133 |
| H | -4.244619 | -4.362846 | -1.626884 |
| O | 8.219172 | 2.53828 | 0.000109 |

| | | | |
|---|---|---|---|
| F | 14.583108 | 2.198757 | -0.642807 |
| S | -5.391177 | 0.606955 | 0.052214 |
| S | 5.262742 | -1.725802 | -0.03732 |
| C | -8.010976 | -0.905382 | -0.092701 |
| H | -8.370759 | -1.923623 | -0.177569 |
| C | -8.984705 | 0.070919 | -0.0232 |
| C | -10.430758 | -0.135329 | -0.052439 |
| C | -8.738933 | 1.52272 | 0.086105 |
| C | -11.066759 | 1.207393 | 0.028001 |
| C | -10.058937 | 2.18195 | 0.111772 |
| C | -12.40378 | 1.603566 | 0.031003 |
| C | -12.66214 | 2.966868 | 0.119038 |
| H | -13.237685 | 0.922011 | -0.030874 |
| C | -10.340353 | 3.537599 | 0.199812 |
| C | -11.672283 | 3.941116 | 0.203716 |
| H | -9.53603 | 4.260073 | 0.263337 |
| H | -11.956012 | 4.983531 | 0.269885 |
| C | -11.130418 | -1.324589 | -0.133509 |
| C | -12.552876 | -1.401096 | -0.153916 |
| N | -13.703429 | -1.520725 | -0.175179 |
| C | -10.52643 | -2.613069 | -0.203835 |
| N | -10.088776 | -3.682778 | -0.26242 |
| O | -7.656332 | 2.090688 | 0.144321 |
| F | -13.949869 | 3.363932 | 0.122421 |

**Table S2**: Cartesian coordinates of **NBD1** compound.

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | -2.160013 | -2.180351 | -0.139343 |
| C | -0.825699 | -2.47144 | -0.147357 |
| C | 0.138902 | -1.424415 | -0.048407 |
| C | -0.304583 | -0.05726 | 0.060033 |
| C | -1.690264 | 0.220766 | 0.067285 |
| H | 1.859378 | -2.73077 | -0.136311 |
| H | -0.472471 | -3.494311 | -0.228701 |
| C | 1.524521 | -1.702583 | -0.054664 |
| C | 0.660026 | 0.989897 | 0.157966 |
| H | -2.024416 | 1.249122 | 0.149845 |
| C | 2.429292 | -0.664517 | 0.042403 |
| H | 0.30681 | 2.01278 | 0.23875 |
| C | 1.99454 | 0.699544 | 0.149651 |
| C | 3.19118 | 1.653356 | 0.243084 |
| C | 4.346057 | 0.66107 | 0.175918 |

| | | | |
|---|---|---|---|
| C | -2.59633 | -0.816741 | -0.030237 |
| C | -4.507791 | -2.138544 | -0.16654 |
| C | -3.356501 | -3.134278 | -0.234538 |
| C | -4.040085 | -0.833867 | -0.049412 |
| C | -5.894411 | -2.260127 | -0.194278 |
| C | -6.616216 | -1.058849 | -0.099972 |
| H | -6.417725 | -3.205436 | -0.282147 |
| C | 3.871533 | -0.642145 | 0.063054 |
| C | 5.734239 | 0.806086 | 0.203863 |
| C | 6.453643 | -0.388951 | 0.112061 |
| H | 6.255369 | 1.748571 | 0.285614 |
| C | 7.832966 | -0.703775 | 0.114316 |
| C | 8.982142 | 0.066158 | 0.124417 |
| C | 9.083486 | 1.543999 | 0.017897 |
| C | 10.346188 | -0.468696 | 0.130198 |
| C | 10.52353 | 1.852932 | -0.138661 |
| C | 11.271866 | 0.669531 | -0.090739 |
| H | 8.010888 | -1.771035 | 0.084103 |
| C | 12.660944 | 0.732569 | -0.232928 |
| C | 13.235892 | 1.979554 | -0.415831 |
| C | 12.473323 | 3.151098 | -0.454196 |
| C | 11.098167 | 3.102304 | -0.31465 |
| H | 13.310966 | -0.128575 | -0.214756 |
| H | 10.502953 | 4.006146 | -0.344445 |
| C | 10.755649 | -1.770083 | 0.353758 |
| C | 9.885128 | -2.850576 | 0.677957 |
| N | 9.229272 | -3.763084 | 0.954431 |
| C | 12.120266 | -2.178057 | 0.319024 |
| N | 13.212272 | -2.55963 | 0.298111 |
| C | 3.19352 | 2.430252 | 1.577422 |
| H | 3.168127 | 1.748879 | 2.430567 |
| H | 4.091519 | 3.048278 | 1.656105 |
| H | 2.323075 | 3.088462 | 1.636145 |
| C | 3.226949 | 2.635822 | -0.947924 |
| H | 2.360421 | 3.301248 | -0.920317 |
| H | 4.128335 | 3.252493 | -0.905518 |
| H | 3.219955 | 2.101076 | -1.900159 |
| C | -3.391868 | -4.118198 | 0.955236 |
| H | -4.291624 | -4.73737 | 0.911497 |
| H | -2.524192 | -4.782184 | 0.928194 |
| H | -3.387119 | -3.584547 | 1.908093 |
| C | -3.357157 | -3.909871 | -1.569587 |
| H | -3.331827 | -3.227581 | -2.422013 |

| | | | |
|---|---|---|---|
| H | -2.486247 | -4.567464 | -1.628738 |
| H | -4.254264 | -4.529165 | -1.650172 |
| O | 8.195551 | 2.380581 | 0.033932 |
| F | 14.564461 | 2.083775 | -0.562082 |
| S | -5.409431 | 0.43416 | 0.042259 |
| S | 5.244661 | -1.888358 | -0.01837 |
| C | -8.028029 | -1.078602 | -0.116481 |
| H | -8.387963 | -2.096344 | -0.20635 |
| C | -9.002402 | -0.102358 | -0.045754 |
| C | -10.44935 | -0.308437 | -0.079269 |
| C | -8.756228 | 1.346318 | 0.071174 |
| C | -11.085289 | 1.031416 | 0.007271 |
| C | -10.079705 | 2.004907 | 0.098063 |
| C | -12.423994 | 1.430867 | 0.010178 |
| C | -12.694763 | 2.78664 | 0.104813 |
| H | -13.259049 | 0.750644 | -0.057084 |
| C | -10.34922 | 3.361407 | 0.19366 |
| C | -11.679025 | 3.742797 | 0.196077 |
| H | -9.559402 | 4.0986 | 0.263501 |
| C | -11.147937 | -1.497632 | -0.168574 |
| C | -12.570387 | -1.571862 | -0.189796 |
| N | -13.721611 | -1.684935 | -0.210405 |
| C | -10.543797 | -2.785487 | -0.246487 |
| N | -10.106029 | -3.854727 | -0.311643 |
| O | -7.677789 | 1.919803 | 0.134633 |
| F | -13.966484 | 3.210523 | 0.110635 |
| F | 13.104033 | 4.319438 | -0.631402 |
| F | -12.021587 | 5.034621 | 0.285419 |

**Table S3**: Cartesian coordinates of **NBD2** compound.

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | -2.178446 | -2.453772 | -0.159041 |
| C | -0.842762 | -2.738344 | -0.165162 |
| C | 0.11629 | -1.687583 | -0.052322 |
| C | -0.33413 | -0.323554 | 0.068426 |
| C | -1.720931 | -0.052248 | 0.073146 |
| H | 1.843369 | -2.984512 | -0.147351 |
| H | -0.484268 | -3.758616 | -0.255171 |
| C | 1.50308 | -1.958933 | -0.056354 |
| C | 0.62482 | 0.727303 | 0.18112 |
| H | -2.06043 | 0.973556 | 0.164694 |
| C | 2.402355 | -0.917311 | 0.055102 |

| | | | |
|---|---|---|---|
| H | 0.266282 | 1.747522 | 0.271097 |
| C | 1.960675 | 0.443489 | 0.175336 |
| C | 3.152052 | 1.402015 | 0.284385 |
| C | 4.312 | 0.416189 | 0.211468 |
| C | -2.621528 | -1.093313 | -0.038141 |
| C | -4.526242 | -2.422912 | -0.194068 |
| C | -3.369945 | -3.412414 | -0.267601 |
| C | -4.064739 | -1.116534 | -0.062713 |
| C | -5.911394 | -2.55021 | -0.227707 |
| C | -6.639188 | -1.35214 | -0.124796 |
| H | -6.430581 | -3.496746 | -0.325925 |
| C | 3.844062 | -0.888646 | 0.081754 |
| C | 5.698524 | 0.567183 | 0.247624 |
| C | 6.424379 | -0.624168 | 0.145452 |
| H | 6.214942 | 1.510977 | 0.342632 |
| C | 7.803785 | -0.932032 | 0.151165 |
| C | 8.950251 | -0.155748 | 0.178354 |
| C | 9.043034 | 1.323001 | 0.08937 |
| C | 10.315723 | -0.685056 | 0.189024 |
| C | 10.484158 | 1.640452 | -0.053559 |
| C | 11.237865 | 0.461342 | -0.014028 |
| H | 7.987855 | -1.997805 | 0.107381 |
| C | 12.622603 | 0.539183 | -0.149637 |
| C | 13.214002 | 1.79263 | -0.317194 |
| C | 12.441694 | 2.965277 | -0.345759 |
| C | 11.057571 | 2.887482 | -0.211847 |
| H | 13.262133 | -0.328764 | -0.136417 |
| H | 10.446307 | 3.78027 | -0.23301 |
| C | 10.730363 | -1.986041 | 0.404897 |
| C | 9.862179 | -3.073115 | 0.713072 |
| N | 9.207677 | -3.990384 | 0.976589 |
| C | 12.097112 | -2.387335 | 0.378524 |
| N | 13.190744 | -2.764493 | 0.364267 |
| C | 3.144775 | 2.164304 | 1.627123 |
| H | 3.118912 | 1.473605 | 2.472711 |
| H | 4.039361 | 2.785765 | 1.716486 |
| H | 2.270892 | 2.817611 | 1.689046 |
| C | 3.188102 | 2.397462 | -0.895832 |
| H | 2.317856 | 3.057839 | -0.864924 |
| H | 4.085905 | 3.018466 | -0.842604 |
| H | 3.18829 | 1.873086 | -1.853833 |
| C | -3.404561 | -4.407812 | 0.912638 |
| H | -4.300803 | -5.031309 | 0.859645 |

| | | | |
|---|---|---|---|
| H | -2.533242 | -5.066839 | 0.882367 |
| H | -3.406099 | -3.883346 | 1.870582 |
| C | -3.362401 | -4.175045 | -1.610091 |
| H | -3.337408 | -3.484481 | -2.455827 |
| H | -2.488163 | -4.827871 | -1.672507 |
| H | -4.256236 | -4.797777 | -1.699686 |
| O | 8.151381 | 2.155348 | 0.107996 |
| S | -5.43893500 | 0.144877 | 0.035495 |
| S | 5.22256400 | -2.127601 | -0.007968 |
| C | -8.049444 | -1.377967 | -0.145753 |
| H | -8.40526 | -2.396283 | -0.244954 |
| C | -9.029134 | -0.405168 | -0.070954 |
| C | -10.47436 | -0.61796 | -0.110675 |
| C | -8.786963 | 1.042654 | 0.053647 |
| C | -11.115695 | 0.721077 | -0.024925 |
| C | -10.114372 | 1.696709 | 0.074757 |
| C | -12.449732 | 1.121521 | -0.029948 |
| C | -12.74618 | 2.482882 | 0.065919 |
| H | -13.269857 | 0.42561 | -0.105833 |
| C | -10.394295 | 3.046122 | 0.171671 |
| C | -11.729022 | 3.445313 | 0.167641 |
| H | -9.597683 | 3.774665 | 0.248116 |
| C | -11.168448 | -1.809583 | -0.20239 |
| C | -12.59044 | -1.890025 | -0.228853 |
| N | -13.74094 | -2.009307 | -0.253822 |
| C | -10.558532 | -3.094949 | -0.276422 |
| N | -10.115284 | -4.162096 | -0.338369 |
| O | -7.711246 | 1.61997 | 0.125956 |
| Cl | 14.94822700 | 1.860421 | -0.490976 |
| Cl | 13.17845600 | 4.531464 | -0.549031 |
| Cl | -12.09710200 | 5.144345 | 0.289047 |
| Cl | -14.42507100 | 2.954791 | 0.055079 |

**Table S4**: Cartesian coordinates of **NBD3** compound.

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | -2.169418 | -2.355205 | -0.154472 |
| C | -0.83422 | -2.641065 | -0.160891 |
| C | 0.125385 | -1.591224 | -0.04426 |
| C | -0.323088 | -0.226494 | 0.081334 |
| C | -1.70902 | 0.046239 | 0.086691 |
| H | 1.850636 | -2.889466 | -0.144753 |
| H | -0.476398 | -3.661144 | -0.25442 |

| | | | |
|---|---|---|---|
| C | 1.511214 | -1.864034 | -0.049962 |
| C | 0.63657 | 0.82345 | 0.197265 |
| H | -2.047731 | 1.071911 | 0.181527 |
| C | 2.411426 | -0.822892 | 0.06424 |
| H | 0.2788 | 1.843515 | 0.290739 |
| C | 1.971999 | 0.53836 | 0.189505 |
| C | 3.164369 | 1.495238 | 0.300007 |
| C | 4.322912 | 0.508331 | 0.22176 |
| C | -2.610471 | -0.994286 | -0.028986 |
| C | -4.516534 | -2.321752 | -0.192966 |
| C | -3.361445 | -3.312258 | -0.267547 |
| C | -4.052653 | -1.014303 | -0.055508 |
| C | -5.899279 | -2.446179 | -0.230453 |
| C | -6.62623 | -1.244689 | -0.124219 |
| H | -6.420642 | -3.390863 | -0.333998 |
| C | 3.85211 | -0.79766 | 0.088488 |
| C | 5.707373 | 0.656059 | 0.254647 |
| C | 6.431515 | -0.539029 | 0.145775 |
| H | 6.225697 | 1.598589 | 0.351222 |
| C | 7.80629 | -0.847816 | 0.144749 |
| C | 8.956488 | -0.069453 | 0.167078 |
| C | 9.046143 | 1.404093 | 0.071365 |
| C | 10.318154 | -0.599952 | 0.175276 |
| C | 10.49065 | 1.724199 | -0.082683 |
| C | 11.243996 | 0.545304 | -0.04308 |
| H | 7.991386 | -1.91322 | 0.096412 |
| C | 12.627513 | 0.617375 | -0.195135 |
| C | 13.22253 | 1.873014 | -0.377767 |
| C | 12.443949 | 3.056038 | -0.402496 |
| C | 11.056007 | 2.973248 | -0.252405 |
| H | 13.262323 | -0.254269 | -0.184483 |
| H | 10.437562 | 3.861239 | -0.271251 |
| C | 10.736964 | -1.896704 | 0.40425 |
| C | 9.869191 | -2.978397 | 0.733067 |
| N | 9.213725 | -3.889586 | 1.013675 |
| C | 12.103338 | -2.299198 | 0.373443 |
| N | 13.196628 | -2.676648 | 0.356094 |
| C | 3.160248 | 2.252748 | 1.645523 |
| H | 3.135618 | 1.559351 | 2.488893 |
| H | 4.055143 | 2.87362 | 1.735012 |
| H | 2.286831 | 2.906184 | 1.710999 |
| C | 3.19981 | 2.494346 | -0.877239 |
| H | 2.330138 | 3.155158 | -0.842729 |

| | | | |
|---|---|---|---|
| H | 4.09798 | 3.114596 | -0.822973 |
| H | 3.198247 | 1.973257 | -1.836994 |
| C | -3.399291 | -4.310379 | 0.910439 |
| H | -4.295905 | -4.932907 | 0.854105 |
| H | -2.528541 | -4.969995 | 0.879718 |
| H | -3.401916 | -3.788422 | 1.869713 |
| C | -3.352973 | -4.071184 | -1.612151 |
| H | -3.326247 | -3.37862 | -2.456151 |
| H | -2.479213 | -4.724491 | -1.674762 |
| H | -4.247053 | -4.693061 | -1.704245 |
| O | 8.160606 | 2.242023 | 0.089402 |
| S | 5.42196400 | 0.249774 | 0.045299 |
| S | 5.22517000 | -2.039661 | -0.008973 |
| C | -8.032239 | -1.268409 | -0.149711 |
| H | -8.391258 | -2.284882 | -0.255348 |
| C | -9.012953 | -0.290897 | -0.072649 |
| C | -10.455351 | -0.501657 | -0.117963 |
| C | -8.765496 | 1.150401 | 0.061702 |
| C | -11.097727 | 0.840362 | -0.02529 |
| C | -10.094396 | 1.812348 | 0.084537 |
| C | -12.432029 | 1.240584 | -0.032504 |
| C | -12.729255 | 2.606422 | 0.07377 |
| H | -13.25006 | 0.543118 | -0.117186 |
| C | -10.36356 | 3.163052 | 0.191767 |
| C | -11.700856 | 3.573093 | 0.18766 |
| H | -9.559825 | 3.882936 | 0.276194 |
| C | -11.155628 | -1.688327 | -0.218423 |
| C | -12.577872 | -1.764751 | -0.248281 |
| N | -13.72843 | -1.881045 | -0.276167 |
| C | -10.549061 | -2.975191 | -0.298709 |
| N | -10.10744 | -4.042437 | -0.365959 |
| O | -7.692666 | 1.730854 | 0.140739 |
| C | 13.06287 | 4.331206 | -0.582654 |
| N | 13.548636 | 5.368522 | -0.727025 |
| C | 14.641272 | 1.944918 | -0.541525 |
| N | 15.786991 | 1.994495 | -0.673518 |
| C | -12.016469 | 4.962093 | 0.298244 |
| N | -12.255866 | 6.087841 | 0.388783 |
| C | -14.099554 | 3.01511 | 0.065641 |
| N | -15.208161 | 3.336786 | 0.058229 |

**Table S5**: Cartesian coordinates of **NBD4** compound.

| Atoms | X-axis | Y-axis | Z-axis |
|---|---|---|---|
| C | 2.187009 | -2.639274 | 0.179363 |
| C | 0.850609 | -2.919614 | 0.17892 |
| C | -0.103667 | -1.867346 | 0.04154 |
| C | 0.351497 | -0.506079 | -0.097554 |
| C | 1.738433 | -0.239098 | -0.095863 |
| H | -1.835232 | -3.156937 | 0.144512 |
| H | 0.487878 | -3.93699 | 0.282268 |
| C | -1.490642 | -2.134225 | 0.039706 |
| C | -0.602582 | 0.546428 | -0.233783 |
| H | 2.082154 | 0.783868 | -0.201101 |
| C | -2.385451 | -1.090662 | -0.094269 |
| H | -0.239764 | 1.563772 | -0.336706 |
| C | -1.939172 | 0.267084 | -0.232847 |
| C | -3.126158 | 1.227793 | -0.364002 |
| C | -4.289668 | 0.247302 | -0.280852 |
| C | 2.634491 | -1.28188 | 0.039667 |
| C | 4.534107 | -2.61482 | 0.233214 |
| C | 3.374308 | -3.59945 | 0.313926 |
| C | 4.076162 | -1.307233 | 0.075975 |
| C | 5.915944 | -2.743838 | 0.279849 |
| C | 6.648071 | -1.546184 | 0.161928 |
| H | 6.433383 | -3.688985 | 0.397759 |
| C | -3.825767 | -1.059457 | -0.129148 |
| C | -5.672901 | 0.401004 | -0.322895 |
| C | -6.403369 | -0.789576 | -0.20378 |
| H | -6.185776 | 1.344988 | -0.43278 |
| C | -7.779341 | -1.09031 | -0.206164 |
| C | -8.924511 | -0.304059 | -0.235552 |
| C | -9.004505 | 1.169495 | -0.13859 |
| C | -10.288895 | -0.826169 | -0.246696 |
| C | -10.448268 | 1.497518 | 0.012937 |
| C | -11.207299 | 0.324558 | -0.026091 |
| H | -7.972008 | -2.154208 | -0.152313 |
| C | -12.593071 | 0.405982 | 0.119922 |
| C | -13.162349 | 1.660235 | 0.302076 |
| C | -12.385361 | 2.822285 | 0.34521 |
| C | -11.008993 | 2.749975 | 0.191327 |
| H | -13.246572 | -0.45176 | 0.096164 |
| H | -10.398447 | 3.642305 | 0.230334 |
| C | -10.717338 | -2.118609 | -0.479065 |
| C | -9.856835 | -3.205044 | -0.81152 |
| N | -9.206854 | -4.119083 | -1.095248 |

| | | | |
|---|---|---|---|
| C | -12.087127 | -2.509467 | -0.448108 |
| N | -13.184288 | -2.8753 | -0.430877 |
| C | -3.109383 | 1.967224 | -1.719521 |
| H | -3.082239 | 1.262491 | -2.553361 |
| H | -4.000703 | 2.590943 | -1.823447 |
| H | -2.232488 | 2.615688 | -1.787746 |
| C | -3.164732 | 2.242663 | 0.799559 |
| H | -2.29135 | 2.8984 | 0.762306 |
| H | -4.059186 | 2.866798 | 0.730719 |
| H | -3.172592 | 1.734491 | 1.766185 |
| C | 3.415667 | -4.614682 | -0.849158 |
| H | 4.308777 | -5.24064 | -0.777481 |
| H | 2.541488 | -5.269566 | -0.814958 |
| H | 3.427531 | -4.106796 | -1.815883 |
| C | 3.353684 | -4.338696 | 1.669405 |
| H | 3.324131 | -3.633793 | 2.503031 |
| H | 2.476822 | -4.987464 | 1.735631 |
| H | 4.244555 | -4.962723 | 1.776604 |
| O | -8.11551 | 2.0032 | -0.153098 |
| Se | 5.450056 | -0.049485 | -0.032657 |
| Se | -5.204948 | -2.293986 | -0.025747 |
| C | 8.053412 | -1.574423 | 0.192198 |
| H | 8.409414 | -2.590516 | 0.311388 |
| C | 9.03758 | -0.600515 | 0.106253 |
| C | 10.478834 | -0.815766 | 0.156153 |
| C | 8.794762 | 0.839929 | -0.04006 |
| C | 11.125133 | 0.524034 | 0.059201 |
| C | 10.126915 | 1.496698 | -0.064852 |
| C | 12.462645 | 0.92123 | 0.064936 |
| C | 12.747254 | 2.276578 | -0.051282 |
| H | 13.288964 | 0.232898 | 0.147197 |
| C | 10.403352 | 2.847986 | -0.175592 |
| C | 11.735276 | 3.234928 | -0.161101 |
| H | 9.61337 | 3.583086 | -0.253854 |
| C | 11.177422 | -2.002378 | 0.26172 |
| C | 12.59967 | -2.078123 | 0.295364 |
| N | 13.750344 | -2.191988 | 0.325485 |
| C | 10.568789 | -3.288255 | 0.34234 |
| N | 10.124547 | -4.354312 | 0.409741 |
| O | 7.725548 | 1.425153 | -0.125877 |
| N | -12.966731 | 4.144257 | 0.659886 |
| O | -13.811161 | 4.186034 | 1.539127 |
| O | -12.521074 | 5.101278 | 0.048384 |

| | | | |
|---|---|---|---|
| N | -14.640763 | 1.717462 | 0.346196 |
| O | -15.17969 | 2.603375 | -0.296108 |
| O | -15.209945 | 0.848444 | 0.985159 |
| N | 12.023308 | 4.684607 | -0.162577 |
| O | 12.873643 | 5.084201 | 0.615228 |
| O | 11.35217 | 5.378042 | -0.908989 |
| N | 14.176305 | 2.647746 | -0.156387 |
| O | 14.955441 | 2.065172 | 0.578917 |
| O | 14.471989 | 3.47645 | -1.001286 |

**Table S6**: Cartesian coordinates of **NBD5** compound.

| **Atoms** | **X-axis** | **Y-axis** | **Z-axis** |
|---|---|---|---|
| C | 2.205403 | -2.894874 | 0.183334 |
| C | 0.86798 | -3.170565 | 0.184852 |
| C | -0.082953 | -2.115474 | 0.046966 |
| C | 0.377057 | -0.756394 | -0.094717 |
| C | 1.765359 | -0.494258 | -0.094345 |
| H | -1.818884 | -3.399241 | 0.153352 |
| H | 0.502039 | -4.186678 | 0.289867 |
| C | -1.47113 | -2.377759 | 0.046522 |
| C | -0.573966 | 0.29871 | -0.232667 |
| H | 2.112438 | 0.527449 | -0.201303 |
| C | -2.362575 | -1.332054 | -0.089319 |
| H | -0.208095 | 1.314788 | -0.337905 |
| C | -1.911604 | 0.023643 | -0.231113 |
| C | -3.095897 | 0.987586 | -0.365266 |
| C | -4.262677 | 0.010749 | -0.281356 |
| C | 2.658071 | -1.539505 | 0.04171 |
| C | 4.552694 | -2.879175 | 0.234603 |
| C | 3.38929 | -3.859364 | 0.317215 |
| C | 4.100424 | -1.571123 | 0.076923 |
| C | 5.935376 | -3.014473 | 0.280266 |
| C | 6.672091 | -1.821653 | 0.161728 |
| H | 6.448241 | -3.962145 | 0.398286 |
| C | -3.803318 | -1.295545 | -0.125036 |
| C | -5.646866 | 0.168721 | -0.327799 |
| C | -6.380594 | -1.017798 | -0.20713 |
| H | -6.157215 | 1.113532 | -0.443067 |
| C | -7.759566 | -1.316558 | -0.21242 |
| C | -8.902245 | -0.531688 | -0.256899 |
| C | -8.984652 | 0.94669 | -0.192283 |
| C | -10.269216 | -1.052186 | -0.263075 |

| | | | |
|---|---|---|---|
| C | -10.427354 | 1.27536 | -0.053976 |
| C | -11.184976 | 0.105629 | -0.074134 |
| H | -7.952207 | -2.37989 | -0.148562 |
| C | -12.568501 | 0.19948 | 0.070633 |
| C | -13.166213 | 1.452757 | 0.227937 |
| C | -12.383715 | 2.629081 | 0.222756 |
| C | -10.999866 | 2.525763 | 0.085163 |
| H | -13.199931 | -0.67306 | 0.07678 |
| H | -10.374589 | 3.407721 | 0.084795 |
| C | -10.696183 | -2.349802 | -0.468123 |
| C | -9.835265 | -3.446374 | -0.76456 |
| N | -9.185649 | -4.369652 | -1.018125 |
| C | -12.066569 | -2.739817 | -0.442895 |
| N | -13.162144 | -3.11082 | -0.430239 |
| C | -3.075463 | 1.724685 | -1.721927 |
| H | -3.049174 | 1.018312 | -2.554433 |
| H | -3.965151 | 2.350412 | -1.828186 |
| H | -2.196817 | 2.370829 | -1.790501 |
| C | -3.132466 | 2.004816 | 0.79627 |
| H | -2.256909 | 2.657734 | 0.75901 |
| H | -4.024955 | 2.631617 | 0.725411 |
| H | -3.143089 | 1.498347 | 1.763788 |
| C | 3.425231 | -4.875527 | -0.845211 |
| H | 4.315975 | -5.505024 | -0.774317 |
| H | 2.548443 | -5.526939 | -0.809933 |
| H | 3.438146 | -4.368128 | -1.812205 |
| C | 3.367302 | -4.597984 | 1.672971 |
| H | 3.341167 | -3.892464 | 2.506215 |
| H | 2.488202 | -5.243648 | 1.740674 |
| H | 4.256125 | -5.225078 | 1.779731 |
| O | -8.091524 | 1.776239 | -0.223517 |
| S | 5.48175800 | -0.319922 | -0.033219 |
| S | -5.18787900 | -2.52503 | -0.019898 |
| C | 8.079643 | -1.856153 | 0.192511 |
| H | 8.429494 | -2.874518 | 0.310829 |
| C | 9.067108 | -0.888755 | 0.109605 |
| C | 10.508959 | -1.10992 | 0.162189 |
| C | 8.833732 | 0.556512 | -0.034322 |
| C | 11.158784 | 0.228264 | 0.07298 |
| C | 10.168462 | 1.203823 | -0.047561 |
| C | 12.493614 | 0.628122 | 0.095053 |
| C | 12.814131 | 1.985086 | -0.005278 |
| H | 13.297621 | -0.081561 | 0.195601 |

| | | | |
|---|---|---|---|
| C | 10.463994 | 2.549574 | -0.156518 |
| C | 11.798126 | 2.95649 | -0.143345 |
| H | 9.665044 | 3.271394 | -0.254114 |
| C | 11.199228 | -2.301967 | 0.262085 |
| C | 12.621017 | -2.389035 | 0.295998 |
| N | 13.77023 | -2.5174 | 0.326929 |
| C | 10.583007 | -3.584786 | 0.335062 |
| N | 10.133225 | -4.649031 | 0.396285 |
| O | 7.764958 | 1.142785 | -0.125258 |
| C | 12.059698 | 4.449982 | -0.233868 |
| C | 14.295575 | 2.326665 | -0.00609 |
| C | -12.950673 | 4.025396 | 0.411609 |
| C | -14.681638 | 1.463679 | 0.350798 |
| F | -14.064092 | 4.238417 | -0.314413 |
| F | -13.253238 | 4.26984 | 1.703398 |
| F | -12.058579 | 4.966961 | 0.039317 |
| F | -15.271167 | 1.834987 | -0.804274 |
| F | -15.114577 | 2.298098 | 1.315134 |
| F | -15.161363 | 0.240282 | 0.654075 |
| F | 13.067784 | 4.751806 | -1.073432 |
| F | 14.742874 | 2.592486 | -1.250616 |
| F | 14.579453 | 3.393663 | 0.76494 |
| F | 15.038422 | 1.303141 | 0.461685 |
| F | 12.359652 | 4.978118 | 0.970614 |
| F | 10.97081 | 5.107819 | -0.683832 |

**Table S7**: Cartesian coordinates of **NBD6** compound.

| Atoms | X-axis | Y-axis | Z-axis |
|---|---|---|---|
| C | 2.212765 | -3.101562 | 0.19305 |
| C | 0.874544 | -3.372873 | 0.189487 |
| C | -0.072342 | -2.313589 | 0.055985 |
| C | 0.392017 | -0.954568 | -0.074389 |
| C | 1.780729 | -0.696919 | -0.069562 |
| H | -1.812314 | -3.592799 | 0.145516 |
| H | 0.504924 | -4.388355 | 0.286669 |
| C | -1.460962 | -2.571661 | 0.048213 |
| C | -0.55506 | 0.104878 | -0.206548 |
| H | 2.131516 | 0.324223 | -0.168936 |
| C | -2.348587 | -1.521809 | -0.083094 |
| H | -0.185544 | 1.120486 | -0.302443 |
| C | -1.893418 | -0.166035 | -0.211471 |
| C | -3.074198 | 0.802604 | -0.341569 |

| | | | |
|---|---|---|---|
| C | -4.243912 | -0.171732 | -0.272478 |
| C | 2.669656 | -1.746579 | 0.060647 |
| C | 4.559769 | -3.0942 | 0.246505 |
| C | 3.393048 | -4.070753 | 0.323516 |
| C | 4.111107 | -1.782299 | 0.096249 |
| C | 5.940348 | -3.233632 | 0.290879 |
| C | 6.681296 | -2.04066 | 0.178004 |
| H | 6.450948 | -4.183111 | 0.403686 |
| C | -3.788489 | -1.481881 | -0.126039 |
| C | -5.626123 | -0.010244 | -0.324944 |
| C | -6.363775 | -1.197672 | -0.221205 |
| H | -6.132898 | 0.937267 | -0.432711 |
| C | -7.741157 | -1.492523 | -0.243303 |
| C | -8.882599 | -0.701966 | -0.287487 |
| C | -8.958008 | 0.771719 | -0.187528 |
| C | -10.249666 | -1.217718 | -0.327144 |
| C | -10.403521 | 1.103801 | -0.067497 |
| C | -11.16632 | -0.060207 | -0.129786 |
| H | -7.938518 | -2.555889 | -0.19741 |
| C | -12.554554 | 0.033225 | -0.009563 |
| C | -13.142959 | 1.285312 | 0.164622 |
| C | -12.351174 | 2.452599 | 0.213755 |
| C | -10.966503 | 2.355824 | 0.102794 |
| H | -13.202479 | -0.829027 | -0.038583 |
| H | -10.340714 | 3.236539 | 0.161482 |
| C | -10.680008 | -2.507821 | -0.565251 |
| C | -9.817404 | -3.601052 | -0.870036 |
| N | -9.165738 | -4.52036 | -1.13192 |
| C | -12.051656 | -2.894432 | -0.569021 |
| N | -13.146596 | -3.266719 | -0.58152 |
| C | -3.045863 | 1.552666 | -1.690978 |
| H | -3.017295 | 0.854467 | -2.530259 |
| H | -3.933573 | 2.181521 | -1.795029 |
| H | -2.165503 | 2.197444 | -1.748985 |
| C | -3.113154 | 1.808451 | 0.829821 |
| H | -2.235607 | 2.459089 | 0.802537 |
| H | -4.00349 | 2.438489 | 0.761057 |
| H | -3.129464 | 1.292677 | 1.792296 |
| C | 3.426777 | -5.081924 | -0.843281 |
| H | 4.314839 | -5.715273 | -0.77374 |
| H | 2.547407 | -5.729941 | -0.811668 |
| H | 3.44289 | -4.570575 | -1.808117 |
| C | 3.367461 | -4.814836 | 1.676328 |

| | | | |
|---|---|---|---|
| H | 3.342734 | -4.112805 | 2.51253 |
| H | 2.486206 | -5.457862 | 1.740219 |
| H | 4.254095 | -5.445264 | 1.781139 |
| O | -8.065384 | 1.60189 | -0.180413 |
| Se | 5.494022 | -0.534186 | -0.008091 |
| Se | -5.175035 | -2.709436 | -0.04196 |
| C | 8.08591 | -2.079781 | 0.207867 |
| H | 8.434087 | -3.099146 | 0.321839 |
| C | 9.077884 | -1.112812 | 0.12678 |
| C | 10.517206 | -1.339169 | 0.17789 |
| C | 8.84614 | 0.329295 | -0.015595 |
| C | 11.173164 | -0.002908 | 0.081481 |
| C | 10.184718 | 0.97517 | -0.0364 |
| C | 12.514271 | 0.38702 | 0.091283 |
| C | 12.820566 | 1.742078 | -0.012204 |
| H | 13.328865 | -0.315993 | 0.173902 |
| C | 10.472954 | 2.325139 | -0.145178 |
| C | 11.807474 | 2.714585 | -0.138084 |
| H | 9.681378 | 3.058548 | -0.228665 |
| C | 11.207057 | -2.530178 | 0.286811 |
| C | 12.628612 | -2.618953 | 0.323449 |
| N | 13.777396 | -2.749112 | 0.357528 |
| C | 10.588146 | -3.811141 | 0.370571 |
| N | 10.135653 | -4.873495 | 0.440816 |
| O | 7.78239 | 0.924162 | -0.10135 |
| O | -14.117173 | 4.089275 | 1.373519 |
| O | -11.8322 | 4.978373 | 0.804633 |
| O | -15.479745 | 2.228274 | -0.681099 |
| O | -15.378185 | -0.139875 | 0.183101 |
| O | 13.113164 | 4.821493 | 0.789928 |
| O | 10.837335 | 5.186232 | -0.221245 |
| O | 15.347302 | 0.901941 | -0.011976 |
| O | 14.80811 | 3.099521 | -1.113713 |
| O | -15.271265 | 1.6976 | 1.766468 |
| O | -13.563786 | 4.579959 | -0.949308 |
| O | 12.728389 | 4.718982 | -1.683294 |
| O | 14.849704 | 2.840189 | 1.37693 |
| H | 14.368096 | 3.702516 | 1.388794 |
| H | 13.610386 | 4.275534 | -1.717888 |
| H | -12.859021 | 4.955575 | -1.503378 |
| H | -15.044449 | 2.651534 | 1.855598 |
| S | -14.963183 | 1.246133 | 0.255612 |
| S | -12.966072 | 4.134563 | 0.480652 |

| | | | |
|---|---|---|---|
| S | 12.106577 | 4.497071 | -0.22655 |
| S | 14.590769 | 2.131438 | -0.033314 |

**Table S8**: Cartesian coordinates of **NBD7** compound.

| Atoms | X-axis | Y-axis | Z-axis |
|---|---|---|---|
| C | -2.213583 | -2.927526 | -0.139369 |
| C | -0.87588 | -3.202333 | -0.135299 |
| C | 0.075067 | -2.142478 | -0.040282 |
| C | -0.385673 | -0.779683 | 0.052431 |
| C | -1.774428 | -0.518431 | 0.045373 |
| H | 1.811804 | -3.428238 | -0.105413 |
| H | -0.509661 | -4.221552 | -0.203207 |
| C | 1.463699 | -2.40371 | -0.034564 |
| C | 0.565168 | 0.280001 | 0.150187 |
| H | -2.121752 | 0.506462 | 0.114893 |
| C | 2.35497 | -1.353595 | 0.060972 |
| H | 0.198927 | 1.299043 | 0.219979 |
| C | 1.903068 | 0.00585 | 0.155707 |
| C | 3.087064 | 0.974744 | 0.253754 |
| C | 4.254362 | -0.00376 | 0.202035 |
| C | -2.666999 | -1.56805 | -0.04887 |
| C | -4.561263 | -2.91471 | -0.182746 |
| C | -3.397661 | -3.897118 | -0.230756 |
| C | -4.109939 | -1.60229 | -0.078651 |
| C | -5.945257 | -3.05323 | -0.217239 |
| C | -6.682174 | -1.858606 | -0.143664 |
| H | -6.457005 | -4.00582 | -0.293399 |
| C | 3.796157 | -1.314176 | 0.091438 |
| C | 5.639231 | 0.15764 | 0.241392 |
| C | 6.374161 | -1.030231 | 0.159043 |
| H | 6.148573 | 1.106368 | 0.324961 |
| C | 7.755144 | -1.327639 | 0.167869 |
| C | 8.896546 | -0.542538 | 0.190979 |
| C | 8.978776 | 0.93559 | 0.106284 |
| C | 10.26605 | -1.062015 | 0.196747 |
| C | 10.418852 | 1.264699 | -0.045711 |
| C | 11.179347 | 0.089743 | -0.019356 |
| H | 7.947586 | -2.392147 | 0.128409 |
| C | 12.558173 | 0.181795 | -0.184306 |
| C | 13.151349 | 1.440447 | -0.350482 |
| C | 12.371889 | 2.613905 | -0.359913 |
| C | 10.984801 | 2.514631 | -0.211533 |

| | | | |
|---|---|---|---|
| H | 13.20873 | -0.678852 | -0.199828 |
| H | 10.352791 | 3.394549 | -0.237199 |
| C | 10.692404 | -2.356342 | 0.424365 |
| C | 9.832865 | -3.446924 | 0.745338 |
| N | 9.184544 | -4.365412 | 1.019517 |
| C | 12.062763 | -2.747136 | 0.40504 |
| N | 13.156752 | -3.123071 | 0.401422 |
| C | 3.068564 | 1.759132 | 1.583583 |
| H | 3.042971 | 1.082455 | 2.440445 |
| H | 3.958839 | 2.387633 | 1.66661 |
| H | 2.190352 | 2.40788 | 1.63045 |
| C | 3.121235 | 1.950689 | -0.942669 |
| H | 2.245749 | 2.604611 | -0.926689 |
| H | 4.013959 | 2.579471 | -0.895557 |
| H | 3.130078 | 1.410505 | -1.89179 |
| C | -3.428914 | -4.866496 | 0.971032 |
| H | -4.320334 | -5.497688 | 0.928779 |
| H | -2.552606 | -5.519415 | 0.958042 |
| H | -3.437693 | -4.321056 | 1.917154 |
| C | -3.380429 | -4.689081 | -1.556039 |
| H | -3.356929 | -4.017237 | -2.416754 |
| H | -2.501865 | -5.337532 | -1.601009 |
| H | -4.269972 | -5.319387 | -1.634697 |
| O | 8.082991 | 1.763474 | 0.134634 |
| S | -5.49392100 | -0.349137 | -0.015846 |
| S | 5.18334800 | -2.544391 | 0.024213 |
| C | -8.092215 | -1.896141 | -0.159863 |
| H | -8.440062 | -2.919429 | -0.232754 |
| C | -9.07908 | -0.929114 | -0.107495 |
| C | -10.522445 | -1.153623 | -0.129548 |
| C | -8.848068 | 0.524551 | -0.042612 |
| C | -11.174064 | 0.184683 | -0.113041 |
| C | -10.180166 | 1.170574 | -0.052697 |
| C | -12.511448 | 0.577427 | -0.145495 |
| C | -12.825719 | 1.939155 | -0.100889 |
| H | -13.322355 | -0.132233 | -0.198157 |
| C | -10.474001 | 2.521057 | -0.029386 |
| C | -11.814312 | 2.918367 | -0.061071 |
| H | -9.680626 | 3.255796 | -0.004433 |
| C | -11.208516 | -2.352924 | -0.140662 |
| C | -12.630007 | -2.449543 | -0.153909 |
| N | -13.778323 | -2.589211 | -0.163482 |
| C | -10.587582 | -3.635388 | -0.127288 |

| | | | |
|---|---|---|---|
| N | -10.134817 | -4.700226 | -0.114916 |
| O | -7.775759 | 1.110938 | 0.006074 |
| O | 13.014642 | 4.372318 | -1.811996 |
| O | 13.201722 | 4.819225 | 0.340863 |
| O | 15.165036 | 2.6612 | -0.343546 |
| O | 15.292097 | 0.454895 | -0.769755 |
| O | -13.180087 | 4.786806 | -0.676077 |
| O | -11.194043 | 5.154016 | 0.31954 |
| O | -15.072347 | 1.902336 | -0.925866 |
| O | -14.62082 | 2.971847 | 1.00941 |
| C | 16.592408 | 2.790318 | -0.534891 |
| H | 16.809636 | 3.841678 | -0.368517 |
| H | 17.123003 | 2.165869 | 0.183473 |
| H | 16.859561 | 2.496248 | -1.549519 |
| C | 13.19732 | 4.3481 | 1.706784 |
| H | 12.203206 | 4.014324 | 2.005338 |
| H | 13.924274 | 3.546512 | 1.8351 |
| H | 13.488563 | 5.208726 | 2.303745 |
| C | -11.403113 | 6.578714 | 0.196131 |
| H | -10.523339 | 7.037459 | 0.638848 |
| H | -11.496086 | 6.855683 | -0.854101 |
| H | -12.303922 | 6.873711 | 0.734239 |
| C | -15.999486 | 3.395234 | 1.102422 |
| H | -16.080832 | 3.901663 | 2.060341 |
| H | -16.231459 | 4.078729 | 0.285223 |
| H | -16.66465 | 2.532834 | 1.063345 |
| C | 12.922995 | 3.989198 | -0.673768 |
| C | 14.640925 | 1.441619 | -0.519946 |
| C | -12.162542 | 4.370811 | -0.171085 |
| C | -14.292476 | 2.281381 | -0.086291 |

**Table S9**: Calculated energy (*E*) and energy gap ($\Delta E$) of HOMO-1/LUMO+1 and HOMO-2/LUMO+2 for the entitled compounds in *eV*.

| Compounds | HOMO-1 | LUMO+1 | $\Delta E$ | HOMO-2 | LUMO+2 | $\Delta E$ |
|---|---|---|---|---|---|---|
| **NBR** | -6.540 | -2.977 | 3.077 | -6.729 | -2.928 | 3.71 |
| **NBD1** | -6.548 | -3.017 | 3.105 | -6.746 | -2.945 | 3.652 |
| **NBD2** | -6.557 | -3.057 | 3.069 | -6.782 | -2.967 | 3.594 |
| **NBD3** | -6.561 | -3.101 | 2.908 | -6.776 | -2.987 | 3.206 |
| **NBD4** | -6.601 | -3.580 | 2.815 | -6.895 | -3.081 | 3.035 |
| **NBD5** | -6.581 | -3.287 | 3.017 | -6.844 | -3.024 | 3.418 |
| **NBD6** | -6.602 | -4.000 | 2.898 | -6.910 | -3.212 | 3.197 |
| **NBD7** | -6.619 | -3.832 | 3.049 | -6.917 | -3.131 | 3.488 |

**Table S10**: Wave length, excitation energy and oscillator strength of **NBR** and **NBD1-NBD7** in solvent phase.

| Compounds | $\lambda$ (*nm*) | *E* (*eV*) | $f_{os}$ | MO contributions |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| | 565.772 | 2.191 | 0.002 | H→L+1 (97%) |
| | 493.054 | 2.515 | 0.010 | H-1→L (88%), H→L+3 (8%) |
| **NBR** | 488.566 | 2.538 | 0.225 | H-2→L (90%), H→L+2 (7%) |
| | 485.372 | 2.554 | 0.110 | H→L+2 (86%), H-2→L (7%), H-1→L+3 (3%) |
| | 458.620 | 2.703 | 0.035 | H→L+3 (83%), H-1→L (9%), H-1→L+2 (3%) |
| | 561.900 | 2.207 | 0.002 | H→L+1 (96%) |
| | 495.062 | 2.504 | 0.179 | H→L+2 (86%), H-1→L (5%), H-1→L+3 (3%) |
| **NBD1** | 491.958 | 2.520 | 0.007 | H-1→L (71%), H→L+3 (18%), H→L+2 (7%) |
| | 489.028 | 2.535 | 0.129 | H-2→L (96%) |
| | 467.174 | 2.654 | 0.034 | H-1→L (21%), H→L+3 (72%) |
| | 568.522 | 2.181 | 0.001 | H→L+1 (97%) |
| | 503.057 | 2.465 | 0.196 | H→L+2 (90%), H-1→L (2%), H-1→L+3 (3%) |
| **NBD2** | 498.105 | 2.489 | 0.003 | H-1→L (72%), H→L+3 (21%), H→L+2 (3%) |
| | 495.695 | 2.501 | 0.126 | H-2→L (96%) |
| | 475.433 | 2.608 | 0.046 | H-1→L (23%), H→L+3 (71%) |
| | 618.371 | 2.005 | 0.007 | H→L+1 (96%) |
| | 577.042 | 2.149 | 0.351 | H→L+2 (96%), H-1→L+3 (2%) |
| **NBD3** | 534.918 | 2.318 | 0.031 | H-1→L (22%), H→L+3 (74%) |
| | 518.824 | 2.390 | 0.160 | H-2→L (96%) |
| | 503.281 | 2.464 | 0.012 | H-1→L (76%), H→L+3 (21%) |
| | 653.645 | 1.897 | 0.022 | H→L+1 (96%) |
| | 619.855 | 2.000 | 0.583 | H→L+2 (97%) |
| **NBD4** | 551.503 | 2.248 | 0.025 | H-1→L (12%), H→L+3 (85%) |
| | 522.894 | 2.371 | 0.162 | H-2→L (94%), H-2→L+2 (3%) |
| | 510.240 | 2.430 | 0.002 | H-1→L (85%), H→L+3 (13%) |
| | 584.551 | 2.121 | 0.004 | H→L+1 (96%) |
| | 531.935 | 2.331 | 0.222 | H→L+2 (95%), H-1→L+3 (3%) |
| **NBD5** | 510.409 | 2.429 | 0.025 | H-1→L (45%), H→L+3 (51%) |
| | 505.931 | 2.451 | 0.148 | H-2→L (96%) |
| | 487.759 | 2.542 | 0.022 | H-1→L (53%), H→L+3 (43%) |
| | 623.847 | 1.987 | 0.022 | H→L+1 (95%) |
| | 578.146 | 2.145 | 0.394 | H→L+2 (96%), H-1→L+3 (2%) |
| **NBD6** | 532.026 | 2.330 | 0.032 | H-1→L (27%), H→L+3 (69%) |
| | 520.588 | 2.382 | 0.163 | H-2→L (96%) |
| | 502.099 | 2.469 | 0.011 | H-1→L (71%), H→L+3 (27%) |
| | 574.396 | 2.159 | 0.014 | H→L+1 (96%) |
| | 521.114 | 2.379 | 0.146 | H→L+2 (94%) |
| **NBD7** | 504.120 | 2.459 | 0.046 | H-1→L (50%), H→L+3 (47%) |
| | 497.206 | 2.494 | 0.152 | H-2→L (96%) |
| | 484.102 | 2.561 | 0.033 | H-1→L (48%), H→L+3 (47%), H→L+1 (2%) |

MO=molecular orbital, H=HOMO, L=LUMO, $f_{os}$= oscillator strength, wavelength= $\lambda$ (*nm*)

**Table S11:** Wave length, excitation energy and oscillator strength of **NBR** and **NBD1-NBD7** in gas phase.

| **Compounds** | $\lambda$ (*nm*) | *E* (*eV*) | $f_{os}$ | **MO contributions** |
|---|---|---|---|---|
| | 541.412 | 2.290 | 0.002 | H-1→L (10%), H→L+1 (88%) |
| | 474.777 | 2.611 | 0.025 | H-1→L (65%), H→L+3 (20%), H→L+1 (4%), H→L+2 (6%) |
| **NBR** | 468.888 | 2.644 | 0.221 | H-2→L (13%), H→L+2 (74%), H-1→L (4%), H-1→L+3 (3%) |
| | 464.218 | 2.671 | 0.031 | H-2→L (83%), H→L+2 (11%) |
| | 441.379 | 2.809 | 0.016 | H-1→L (20%), H→L+3 (68%), H→L+1 (5%) |
| | 536.841 | 2.310 | 0.002 | H-1→L (10%), H→L+1 (87%) |

| | | | | |
|---|---|---|---|---|
| | 477.962 | 2.594 | 0.094 | H-1→L (24%), H→L+2 (55%), H→L+3 (13%) |
| **NBD1** | 474.015 | 2.616 | 0.058 | H-1→L (29%), H→L+2 (35%), H→L+3 (27%) |
| | 465.858 | 2.661 | 0.088 | H-2→L (95%) |
| | 446.996 | 2.774 | 0.014 | H-1→L (36%), H→L+3 (50%), H→L+1 (8%) |
| | 541.838 | 2.288 | 0.002 | H-1→L (11%), H→L+1 (87%) |
| | 483.027 | 2.567 | 0.106 | H-1→L (20%), H→L+2 (62%), H→L+3 (11%) |
| **NBD2** | 478.700 | 2.590 | 0.050 | H-1→L (32%), H→L+2 (29%), H→L+3 (30%), H→L+1 (2%) |
| | 470.079 | 2.638 | 0.086 | H-2→L (94%) |
| | 453.073 | 2.737 | 0.022 | H-1→L (37%), H→L+3 (49%), H→L+1 (8%) |
| | 573.254 | 2.163 | 0.003 | H→L+1 (89%), H-1→L (4%), H→L+3 (3%) |
| | 537.352 | 2.307 | 0.234 | H→L+2 (95%), H-1→L+3 (2%) |
| **NBD3** | 516.877 | 2.399 | 0.018 | H-1→L (29%), H→L+3 (68%) |
| | 488.835 | 2.536 | 0.115 | H-2→L (96%) |
| | 471.437 | 2.630 | 0.013 | H-1→L (65%), H→L+3 (26%), H→L+1 (7%) |
| | 588.100 | 2.108 | 0.015 | H→L+1 (91%), H-1→L+2 (2%), H→L+3 (4%) |
| | 559.946 | 2.214 | 0.307 | H→L+2 (95%) |
| **NBD4** | 527.207 | 2.352 | 0.017 | H-1→L (27%), H→L+3 (69%) |
| | 490.770 | 2.526 | 0.120 | H-2→L (96%) |
| | 474.106 | 2.615 | 0.007 | H-1→L (69%), H→L+3 (24%), H→L+1 (4%) |
| | 552.609 | 2.244 | 0.002 | H→L+1 (88%), H-1→L (8%) |
| | 505.910 | 2.451 | 0.166 | H→L+2 (93%), H-1→L+3 (2%) |
| **NBD5** | 494.884 | 2.505 | 0.020 | H-1→L (34%), H→L+3 (60%) |
| | 478.959 | 2.589 | 0.104 | H-2→L (96%) |
| | 460.494 | 2.692 | 0.013 | H-1→L (54%), H→L+3 (33%), H→L+1 (9%) |
| | 580.148 | 2.137 | 0.035 | H→L+1 (90%), H-1→L (3%), H→L+2 (2%), H→L+3 (3%) |
| | 543.834 | 2.280 | 0.249 | H→L+2 (92%), H-1→L (2%) |
| **NBD6** | 516.619 | 2.400 | 0.036 | H-1→L (31%), H→L+3 (66%) |
| | 490.130 | 2.530 | 0.116 | H-2→L (96%) |
| | 471.205 | 2.631 | 0.012 | H-1→L (62%), H→L+3 (27%), H→L+1 (6%), H→L+2 (2%) |
| | 543.001 | 2.283 | 0.000 | H-1→L (10%), H→L+1 (87%) |
| | 494.273 | 2.508 | 0.080 | H→L+2 (93%), H-1→L+2 (2%) |
| **NBD7** | 485.828 | 2.552 | 0.074 | H-1→L (40%), H→L+3 (54%) |
| | 468.782 | 2.645 | 0.098 | H-2→L (95%) |
| | 457.486 | 2.710 | 0.022 | H-1→L (47%), H→L+1 (10%), H→L+3 (39%) |

MO=molecular orbital, H=HOMO, L=LUMO, $f_{os}$= oscillator strength, wavelength= $\lambda$ (*nm*)

**Table S12**: Percentages for HOMOs and LUMOs of the studied compounds.

| | **LUMO** | | **HOMO** | |
|---|---|---|---|---|
| **Compound** | **Acceptor (%)** | **Donor (%)** | **Acceptor (%)** | **Donor (%)** |
| **NBR** | 61.1 | 38.9 | 30.0 | 70.0 |
| **NBD1** | 60.0 | 40.0 | 29.7 | 70.3 |
| **NBD2** | 60.5 | 39.5 | 30.4 | 69.6 |
| **NBD3** | 65.0 | 35.0 | 31.5 | 68.5 |
| **NBD4** | 69.6 | 30.4 | 31.5 | 68.5 |
| **NBD5** | 61.7 | 38.3 | 30.8 | 69.2 |
| **NBD6** | 65.7 | 34.3 | 31.5 | 68.5 |
| **NBD7** | 61.1 | 38.9 | 30.5 | 69.5 |

**Table S13:** Open circuit voltage ($V_{oc}$), Band Gap($\Delta E$), $eV_{oc}/K_BT$, FF, $L_D$-$L_A$($eV$) & PCE (%) of entitled compounds.

| Compounds | $V_{oc}$ | $\Delta E$ | $eV_{oc}/K_BT$ | FF | PCE (%) |
|---|---|---|---|---|---|
| **NBR** | 2.109 | 2.147 | 81.429 | 0.965 | 29.86 |
| **NBD1** | 2.143 | 2.157 | 82.741 | 0.965 | 30.34 |
| **NBD2** | 2.176 | 2.130 | 84.015 | 0.966 | 30.84 |
| **NBD3** | 2.329 | 2.045 | 89.92 | 0.975 | 33.31 |
| **NBD4** | 2.347 | 2.024 | 90.618 | 0.968 | 33.33 |
| **NBD5** | 2.257 | 2.100 | 87.143 | 0.967 | 30.02 |
| **NBD6** | 2.348 | 2.044 | 90.656 | 0.968 | 33.34 |
| **NBD7** | 2.178 | 2.123 | 84.093 | 0.966 | 30.86 |

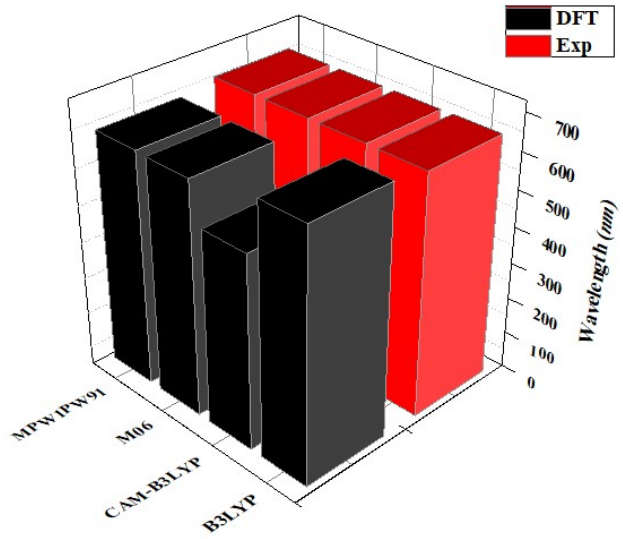
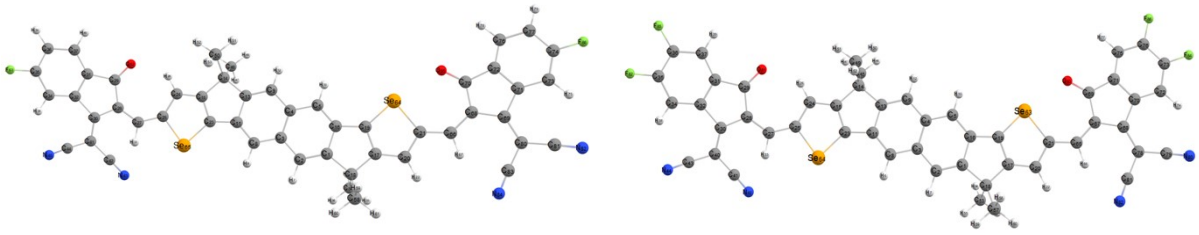
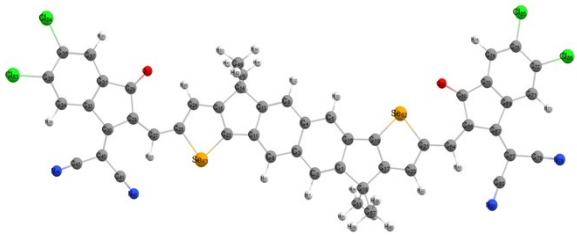


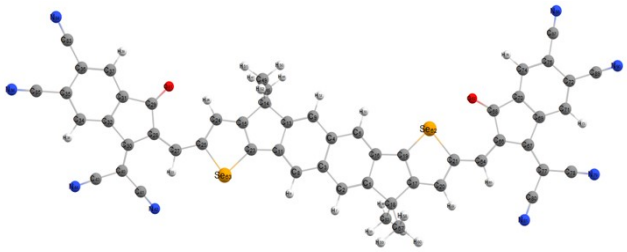

**Figure S1**: A comparative UV–Vis analysis between experimental and DFT-based data of **NBR** compound in chloroform solvent.



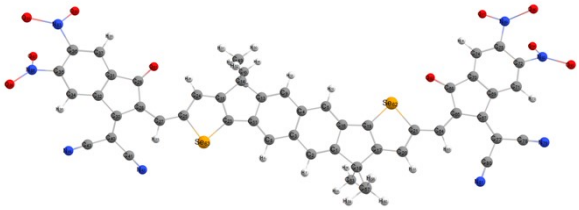
**NBR** **NBD1**



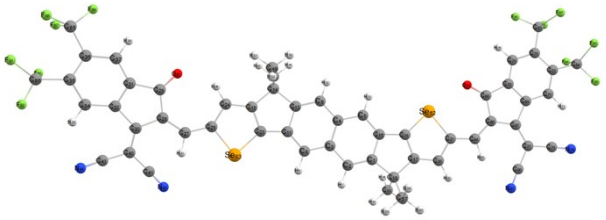
**NBD2**



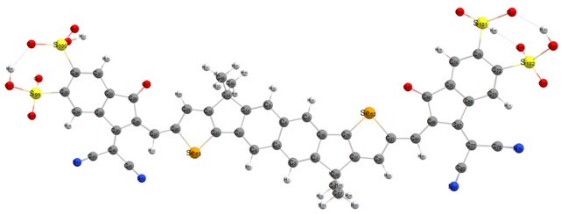
**NBD3**



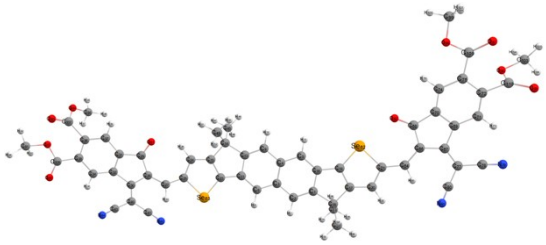
**NBD4**



**NBD5**

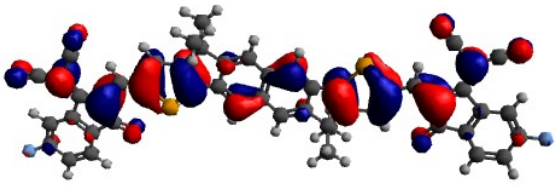


**NBD6**

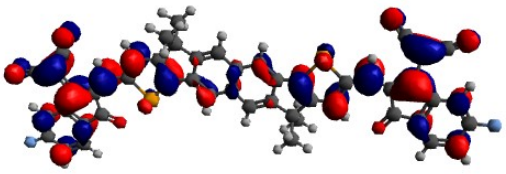


**NBD7**

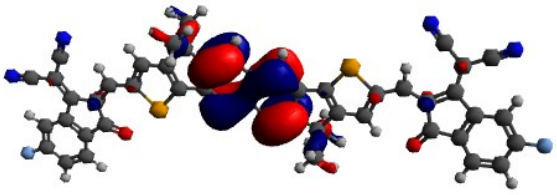
**Figure S2**: The optimized structures of the investigated compounds **NBR** and **NBD1-NBD7.**



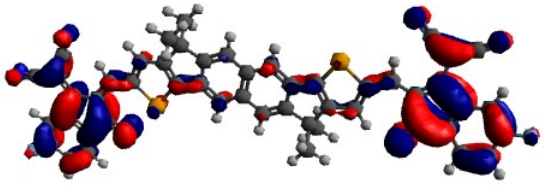
**HOMO-1**



**LUMO+1**

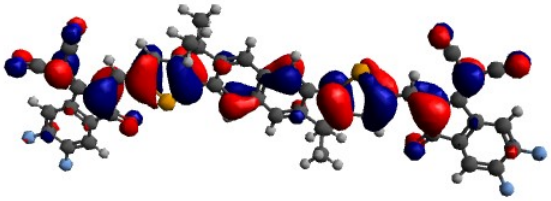


**HOMO-2**

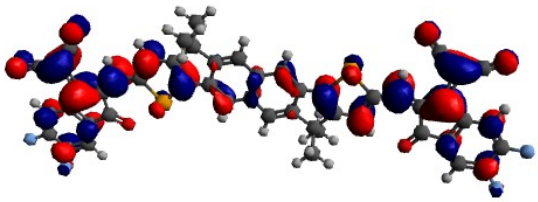


**LUMO+2**

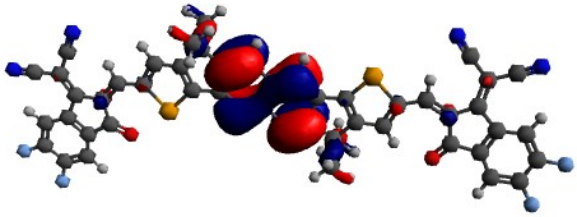
**NBR**



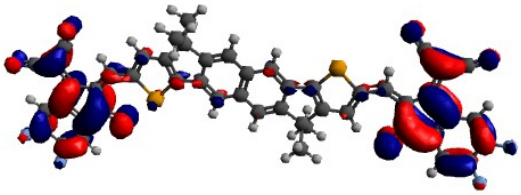
HOMO-1



LUMO+1

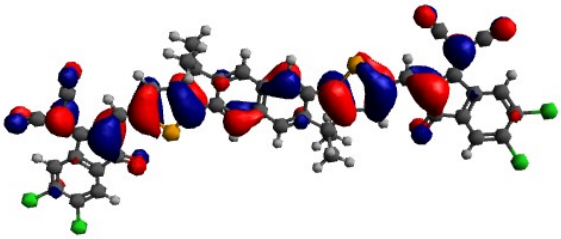


HOMO-2



LUMO+2

NBD1



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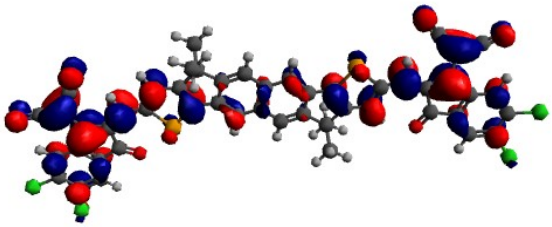
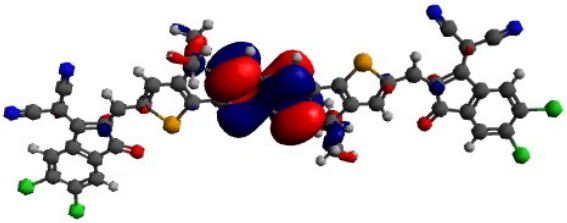


LUMO+1



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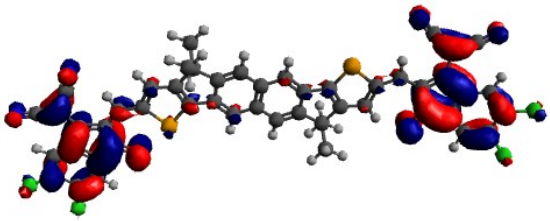
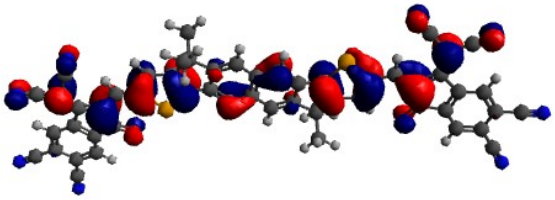
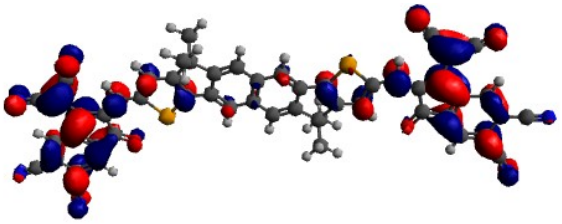


LUMO+2

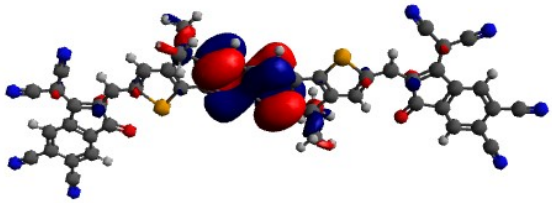
NBD2



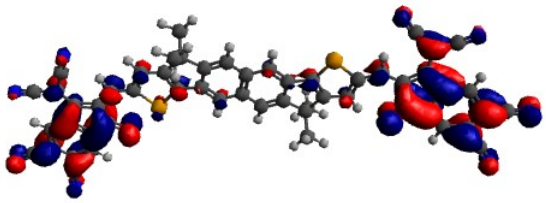
HOMO-1



LUMO+1

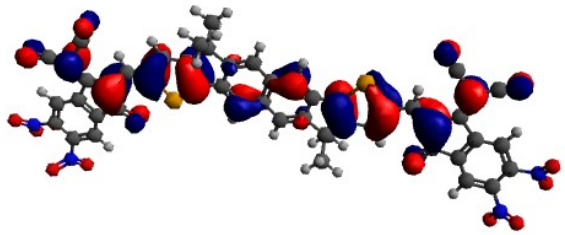


HOMO-2

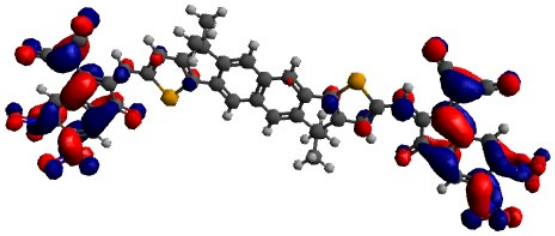


LUMO+2

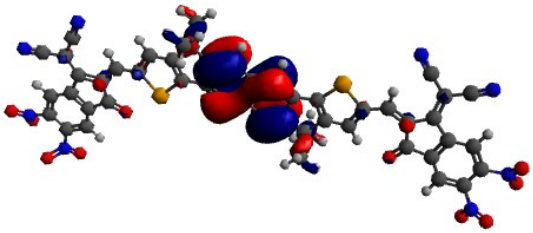
NBD3



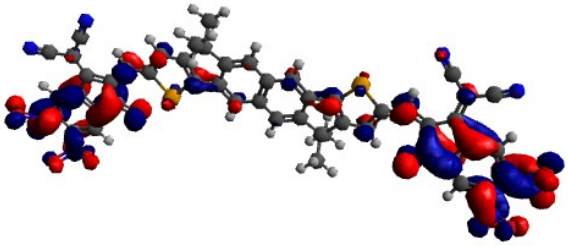
**HOMO-1**



**LUMO+1**

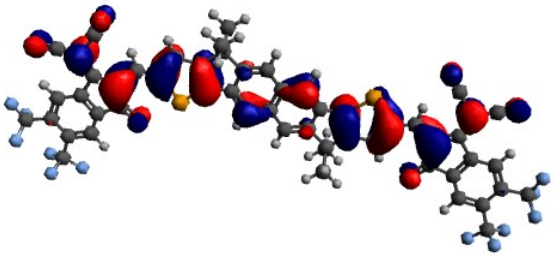


**HOMO-2**

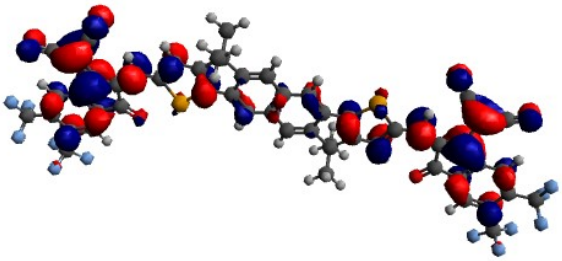


**LUMO+2**

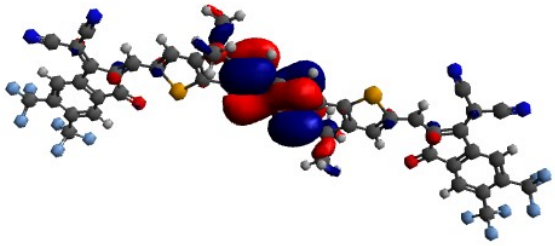
**NBD4**



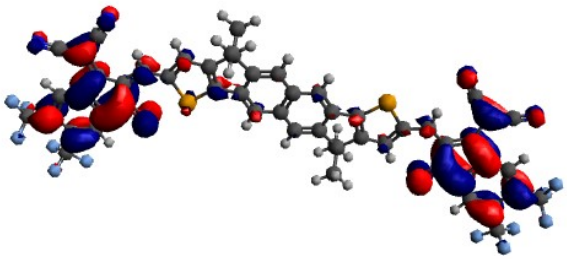
**HOMO-1**



**LUMO+1**

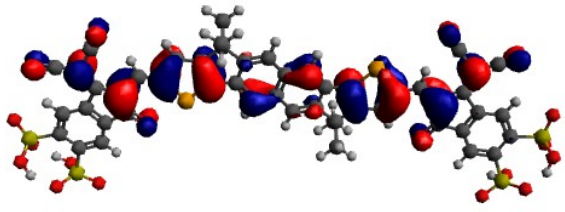


**HOMO-2**

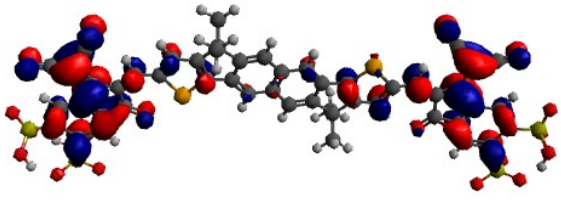


**LUMO+2**

**NBD5**



**HOMO-1**



**LUMO+1**

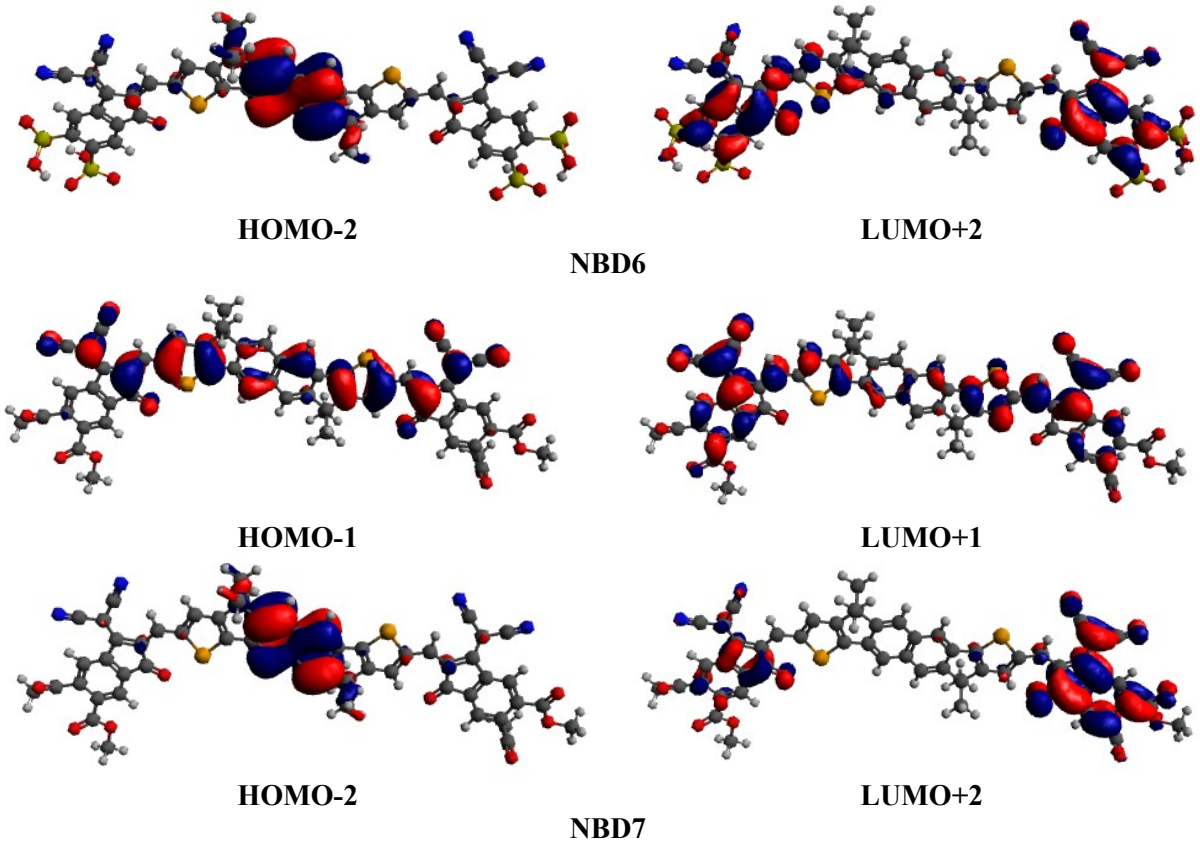



**Figure S3**: Frontier molecular orbital contour plots of HOMO+1/LUMO-1 and HOMO+2/LUMO-2 for the reference (**NBR**) and designed molecules (**NBD1-NBD7**).

$$IP = -E_{HOMO} \quad \text{(S1)}$$

$$EA = -E_{LUMO} \quad \text{(S2)}$$

$$X = \frac{[IP + EA]}{2} \quad \text{(S3)}$$

$$\eta = \frac{[IP - EA]}{2} \quad \text{(S4)}$$

$$\mu = \frac{E_{HOMO} + E_{LUMO}}{2} \quad \text{(S5)}$$

$$\omega = \frac{\mu^2}{2\eta} \quad \text{(S6)}$$

$$\sigma = \frac{1}{2\eta} \tag{S7}$$

$$\Delta Nmax = \frac{\mu}{\eta} \tag{S8}$$