

# Supplementary Materials for DELFI: A computer oracle for recommending density functionals for excited states calculations

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# 1 Pairwise similarity matrix

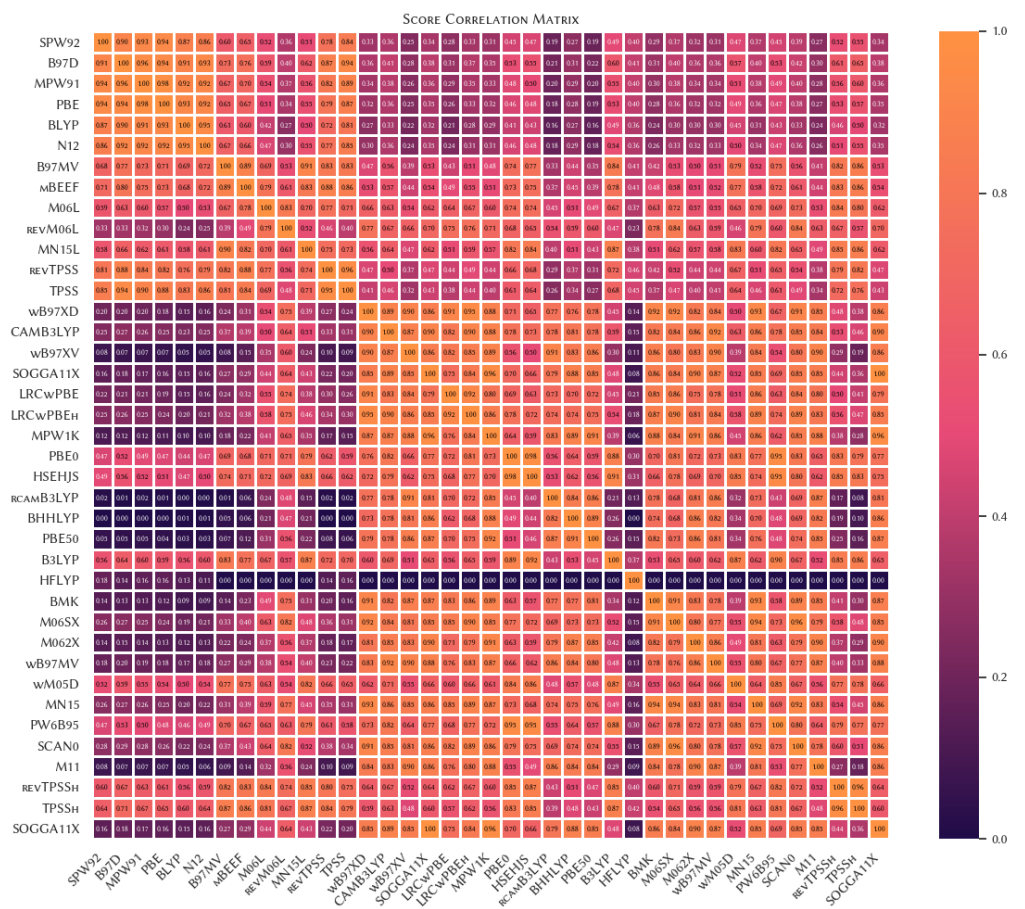


Figure 1: Pairwise similarity of the scores calculated for the functionals selected on QM8 database.

# 2 Model performances on single regression tasks

| Functional | R-2  | MSE  | Uncertainty |
|------------|------|------|-------------|
| SPW92      | 0.74 | 0.14 | 5.3         |
| B97D       | 0.76 | 0.18 | 2.4         |
| MPW91      | 0.74 | 0.16 | 2.4         |
| PBE        | 0.75 | 0.15 | 1.1         |
| BLYP       | 0.75 | 0.12 | 0.8         |
| N12        | 0.74 | 0.15 | 0.8         |
| B97MV      | 0.77 | 0.46 | 1.6         |
| mBEEF      | 0.78 | 0.42 | 1.2         |
| M06L       | 0.76 | 0.56 | 1.4         |
| revM06L    | 0.78 | 0.9  | 2.1         |
| MN15L      | 0.76 | 0.64 | 1.6         |
| revTPSS    | 0.77 | 0.32 | 0.8         |
| TPSS       | 0.77 | 0.26 | 0.7         |
| wB97XD     | 0.67 | 1.24 | 2.3         |
| CAMB3LYP   | 0.63 | 1.15 | 2.0         |
| wB97XV     | 0.64 | 1.38 | 2.3         |
| LRCwPBE    | 0.64 | 1.38 | 2.1         |
| LRCwPBEh   | 0.65 | 1.19 | 1.8         |
| MPW1K      | 0.67 | 1.08 | 1.8         |
| PBE0       | 0.68 | 0.84 | 1.4         |
| HSEHJS     | 0.70 | 0.79 | 1.4         |
| rcamB3LYP  | 0.63 | 1.32 | 1.8         |
| BHHLYP     | 0.64 | 1.09 | 1.5         |
| PBE50      | 0.64 | 1.14 | 1.4         |
| BMK        | 0.68 | 1.14 | 1.6         |
| M06SX      | 0.7  | 1.03 | 1.5         |
| M062X      | 0.6  | 1.06 | 1.4         |
| wB97MV     | 0.62 | 1.2  | 1.6         |
| wM05D      | 0.72 | 0.71 | 1.0         |
| MN15       | 0.70 | 1.08 | 1.5         |
| PW6B95     | 0.67 | 0.82 | 1.1         |
| SCAN0      | 0.71 | 1.01 | 1.4         |
| M11        | 0.59 | 1.24 | 1.5         |
| revTPSSh   | 0.75 | 0.61 | 0.9         |
| TPSSh      | 0.75 | 0.54 | 0.8         |
| B3LYP      | 0.72 | 0.66 | 0.9         |
| HFLYP      | 0.78 | 0.66 | 1.1         |
| SOGGA11X   | 0.64 | 1.06 | 1.2         |

Table 1: R-squared (R-2), mean standard error (MSE) on the test set for each of the individual regression task of the model, and average value of the variance for the predictions for the single molecules in the test set over 500 resamplings each.

### 3 Spyropiran and merocyanine XYZ coordinates used for the in-silico experiment

#### 3.1 SP1

31

C 4.931669 0.951265 0.000041 C 3.470683 0.965964 -.000016 C 2.810149 -.370768 0.000060 C  
3.633589 -1.552247 0.000088 C 4.995030 -1.489327 0.000086 C 5.645086 -.208547 0.000070 C  
1.428963 -.525977 0.000094 C 0.443787 0.484738 0.000071 C -.901143 0.211712 0.000105 C -  
1.619053 -1.134303 0.000156 C -3.083447 -.746677 0.000084 C -3.169141 0.654300 0.000036 N  
-1.872749 1.180256 0.000090 C -4.388068 1.323887 -.000022 C -5.550010 0.542962 -.000038 C  
-5.484551 -.852173 0.000012 C -4.242940 -1.506103 0.000076 O 2.842644 2.040962 0.000071 H  
5.592835 -2.395507 0.000111 H -1.657221 2.167627 -.000107 H -4.195484 -2.592153 0.000113 H  
-6.400223 -1.435749 0.000001 H -6.517999 1.036096 -.000087 H -4.440988 2.408774 -.000055 H  
-1.340932 -1.727774 -.880077 H -1.341002 -1.727674 0.880479 H 0.787968 1.513543 0.000022 H  
1.074004 -1.558764 0.000143 H 3.132153 -2.519165 0.000117 H 6.732900 -.174213 0.000088 H  
5.415843 1.923389 0.000047

#### 3.2 SP2

33

C 0.8768760 2.9914630 1.1492100 C 0.2050370 1.7820590 1.2601730 C -0.0466730 1.0159120 0.1141910  
C 0.3722320 1.4603790 -1.1606460 C 1.0477780 2.6775310 -1.2609110 C 1.2951150 3.4251700 -  
0.1125190 C 0.0461590 0.6230830 -2.3048720 C -0.5108050 -0.5838720 -2.1344190 C -0.7580000  
-1.1725170 -0.7743360 O -0.7399120 -0.1326440 0.2717290 N 0.2107690 -2.2054780 -0.4657940 C  
-0.3647780 -3.1535670 0.3972430 C -1.7622540 -3.0326040 0.3645550 C -2.1136960 -1.9066320 -  
0.5816540 C 0.2628810 -4.1295280 1.1653320 C -0.5468810 -4.9933980 1.9136920 C -1.9382970  
-4.8826680 1.8903040 C -2.5540290 -3.8942970 1.1078250 H 1.1675860 -1.9074370 -0.3179790  
N 2.0059020 4.6973980 -0.2312050 O 2.2078220 5.3417750 0.8001030 O 2.3638520 5.0540780 -  
1.3560170 H -3.6375370 -3.8043500 1.0909210 H -2.5466480 -5.5617100 2.4804230 H -0.0781220  
-5.7602090 2.5247200 H 1.3455610 -4.2191360 1.1893840 H -2.8651070 -1.2079780 -0.2052640 H  
-2.4632640 -2.2915870 -1.5484790 H -0.7493540 -1.2259300 -2.9765790 H 0.2611660 1.0023670  
-3.3006960 H 1.3809930 3.0516700 -2.2221080 H 1.0861370 3.6034070 2.0177360 H -0.1361930  
1.4126980 2.2213650

### 3.3 SP3

36// C 0.728812 3.168016 1.123990 C 0.123737 1.926729 1.257652 C -0.062582 1.114779 0.129681  
C 0.358703 1.547473 -1.148650 C 0.967136 2.797239 -1.271684 C 1.148085 3.590469 -0.141670 C  
0.116100 0.657092 -2.272618 C -0.393509 -0.568219 -2.083161 C -0.708206 -1.124694 -0.723467  
O -0.688929 -0.065537 0.312322 N 0.203034 -2.185609 -0.339552 C -0.473479 -3.113976 0.467398  
C -1.861055 -2.932753 0.356789 C -2.105800 -1.790013 -0.598396 C 0.060597 -4.116097 1.274715  
C -0.832064 -4.947308 1.965488 C -2.212262 -4.776460 1.859157 C -2.733840 -3.757272 1.046731  
C 1.619900 -1.925200 -0.170195 N 1.787880 4.896459 -0.283741 O 1.931200 5.580489 0.731927 O  
2.149079 5.241352 -1.411434 H -3.809010 -3.616229 0.965449 H -2.885060 -5.428961 2.407791 H  
-0.434647 -5.733974 2.601468 H 1.132654 -4.251825 1.377488 H -2.837193 -1.053816 -0.255333 H  
-2.429342 -2.152734 -1.582744 H 1.951837 -1.231105 -0.945970 H 1.856689 -1.498277 0.815707 H  
2.182108 -2.856764 -0.290683 H -0.571008 -1.243690 -2.914553 H 0.354640 1.011321 -3.272524 H  
1.300202 3.161140 -2.236896 H 0.884409 3.815261 1.978139 H -0.216213 1.566283 2.222673

### 3.4 SP4

35

C -1.658260 -1.550419 -0.750912 C -1.125182 -0.283933 -0.497598 C -1.924395 0.719190 0.072715  
C -3.263701 0.435424 0.395571 C -3.794093 -0.830299 0.146667 C -2.983084 -1.820562 -0.432452  
C -1.310760 2.022703 0.278445 C 0.007941 2.193189 0.099253 C 0.910062 1.035750 -0.235656 O  
0.165610 -0.036711 -0.880397 N 1.596023 0.553220 0.959900 C 2.831841 -0.002352 0.596876 C  
3.193533 0.443190 -0.684904 C 2.090125 1.340294 -1.198205 C 3.668964 -0.833052 1.337311 C  
4.888261 -1.216029 0.764239 C 5.257988 -0.779497 -0.509183 C 4.403696 0.059282 -1.241136 O  
-5.080688 -1.208465 0.425111 H 1.019422 0.074559 1.642153 H 4.687238 0.397050 -2.235310 H  
6.206941 -1.090980 -0.936100 H 5.553736 -1.868280 1.323974 H 3.385900 -1.178945 2.327976 H  
1.785713 1.146233 -2.229776 H 2.368908 2.399313 -1.119044 H 0.489435 3.152302 0.263597 H -  
1.944072 2.854686 0.578701 H -3.867361 1.220784 0.837938 H -3.414825 -2.798426 -0.620633 H  
-1.024220 -2.307848 -1.200861 C -5.947421 -0.246304 0.998515 H -6.907575 -0.748174 1.133338 H  
-5.580503 0.099814 1.974734 H -6.082961 0.622053 0.339091

### 3.5 SP5

35

C -2.945106 -3.587208 0.998409 C -1.985982 -2.772071 0.414000 C -.625586 -3.078561 0.540750  
C -.195990 -4.211958 1.231034 C -1.175925 -5.022090 1.815292 C -2.534219 -4.720622 1.708134  
C -2.163954 -1.538216 -.429561 C -.739947 -.923409 -.562857 N 0.116791 -2.075097 -.147475 O

-6.28784 0.099215 0.439527 C -.090629 1.320997 0.177649 C 0.186925 1.748346 -1.136250 C -  
.049751 0.807093 -2.216774 C -.446352 -.443543 -1.955397 C 0.681787 3.038603 -1.330400 C 0.889918  
3.867555 -.231709 C 0.616145 3.442448 1.070748 C 0.121571 2.160841 1.274143 N 1.405511 5.220209  
-.448224 O 1.634142 5.568826 -1.608010 N 1.485027 -1.906924 -.027981 O 1.578839 5.933400  
0.541439 H -4.000617 -3.345772 0.904048 H -3.273530 -5.367065 2.171644 H -.861429 -5.905848  
2.363052 H 0.852572 -4.452165 1.317507 H -2.828052 -.788216 0.008421 H -2.553713 -1.788042  
-1.423685 H -.605012 -1.173716 -2.742938 H 0.122780 1.133330 -3.238746 H 0.909036 3.403554  
-2.325253 H 0.793021 4.117279 1.898865 H -.104306 1.794999 2.269841 O 2.132100 -2.854579  
0.410403 O 1.943099 -.830640 -.403298

### 3.6 MC1

31

C 4.931669 0.951265 0.000041 C 3.470683 0.965964 -.000016 C 2.810149 -.370768 0.000060 C  
3.633589 -1.552247 0.000088 C 4.995030 -1.489327 0.000086 C 5.645086 -.208547 0.000070 C  
1.428963 -.525977 0.000094 C 0.443787 0.484738 0.000071 C -.901143 0.211712 0.000105 C -  
1.619053 -1.134303 0.000156 C -3.083447 -.746677 0.000084 C -3.169141 0.654300 0.000036 N  
-1.872749 1.180256 0.000090 C -4.388068 1.323887 -.000022 C -5.550010 0.542962 -.000038 C  
-5.484551 -.852173 0.000012 C -4.242940 -1.506103 0.000076 O 2.842644 2.040962 0.000071 H  
5.592835 -2.395507 0.000111 H -1.657221 2.167627 -.000107 H -4.195484 -2.592153 0.000113 H  
-6.400223 -1.435749 0.000001 H -6.517999 1.036096 -.000087 H -4.440988 2.408774 -.000055 H  
-1.340932 -1.727774 -.880077 H -1.341002 -1.727674 0.880479 H 0.787968 1.513543 0.000022 H  
1.074004 -1.558764 0.000143 H 3.132153 -2.519165 0.000117 H 6.732900 -.174213 0.000088 H  
5.415843 1.923389 0.000047

### 3.7 MC2

33

C 1.7351040 1.2814340 -3.7714520 C 1.7839040 1.3760270 -2.3866180 C 2.7911360 2.1456150 -  
1.7855350 C 3.7592980 2.8264790 -2.5155050 C 3.6924580 2.7232510 -3.9081380 C 2.6946900  
1.9642090 -4.5296040 C 0.9513000 0.7601000 -1.2964800 C 1.5418730 1.3217730 -0.0363950 N  
2.6121460 2.0814830 -0.3949590 O 0.8078440 -1.6551050 0.0316110 C -0.3076130 -1.6436720 0.5970270  
C -0.7288840 -0.5743850 1.5292160 C 0.0412470 0.5613960 1.8679180 C 1.1088800 1.2507130  
1.2867220 C -1.9438840 -0.7434100 2.2533820 C -2.7736760 -1.8097630 2.0190050 C -2.4315740  
-2.8217570 1.0725700 C -1.2502990 -2.7380260 0.4019350 N -4.0214960 -1.9168180 2.7563720  
O -4.2971050 -1.0335590 3.5757510 O -4.7442160 -2.8913240 2.5218040 H 3.2098030 2.5481380  
0.2745580 H 0.9669050 0.6886190 -4.2602330 H 2.6652690 1.9023170 -5.6133320 H 4.4290820

3.2425180 -4.5142400 H 4.5338540 3.4139050 -2.0308780 H 1.0350540 -0.3451290 -1.2293870 H -  
0.1258080 0.9586380 -1.3619850 H 1.6031330 1.9566630 1.9546330 H -0.2612160 1.0058960 2.8175800  
H -2.2449250 -0.0037870 2.9877120 H -3.1200720 -3.6451820 0.9231500 H -0.9478670 -3.5031810  
-0.3062430

### 3.8 MC3

36

C 1.753736 0.207624 -0.015334 C 2.190010 -1.248861 -0.025075 C 3.696223 -1.153725 -0.011637  
C 4.050225 0.202715 -0.007007 N 2.874356 0.985368 -0.027011 C 5.378643 0.615923 0.015040 C  
6.363694 -0.379034 0.023165 C 6.026054 -1.733727 0.012894 C 4.680909 -2.129123 -0.003698 C  
2.847842 2.440434 -0.031992 C 0.467293 0.717319 0.007089 C -0.667573 -0.104092 -0.003506 C  
-2.008004 0.301332 0.008789 C -2.419423 1.733787 0.032309 O -1.608023 2.675353 0.046916 C -  
3.008816 -0.710029 -0.006213 C -4.340577 -0.388335 0.000257 N -5.329975 -1.449805 -0.016262  
O -6.522577 -1.123914 -0.010766 C -4.776653 0.975747 0.022252 C -3.861049 1.979914 0.037186  
O -4.935145 -2.621777 -0.035009 H 4.417544 -3.183535 -0.008502 H 6.808909 -2.485931 0.020482  
H 7.409113 -0.084880 0.040542 H 5.657481 1.664299 0.031743 H 1.792403 -1.783515 0.846350 H  
1.808010 -1.766167 -0.914367 H 2.123191 2.795405 -0.769368 H 2.568506 2.831648 0.952713 H  
3.833918 2.817843 -0.302441 H 0.297617 1.786036 0.037253 H -0.508733 -1.183494 -0.025409 H  
-2.723314 -1.756940 -0.023510 H -5.842363 1.172652 0.026418 H -4.164684 3.021963 0.053995

### 3.9 MC4

35

C -5.119696 -1.353061 0.000063 C -3.950996 -0.608047 0.000021 C -4.018863 0.794177 -0.000055  
C -5.229936 1.478155 -0.000089 C -6.401462 0.711568 -0.000048 C -6.353401 -0.684194 0.000027  
N -2.716727 1.304000 -0.000077 C -1.756307 0.322771 -0.000047 C -2.491591 -1.014235 0.000044  
C -0.409427 0.578991 -0.000096 C 0.564589 -0.444339 -0.000066 C 1.944719 -0.301701 -0.000115  
C 2.629646 1.027845 -0.000220 C 4.077257 0.993447 -0.000024 C 4.787234 -0.177663 0.000020 C  
4.117045 -1.454806 -0.000054 C 2.754752 -1.488337 -0.000090 O 2.006111 2.106958 0.000079 H  
4.684466 -2.377389 -0.000021 H -2.488373 2.288415 -0.000194 H -5.085518 -2.439665 0.000121 H  
-7.276152 -1.256560 0.000058 H -7.363278 1.216697 -0.000075 H -5.269717 2.563617 -0.000146 H  
-2.221549 -1.611263 -0.880280 H -2.221550 -1.611139 0.880454 H -0.049085 1.602480 -0.000167  
H 0.197499 -1.473054 -0.000007 H 2.246864 -2.451496 -0.000078 O 6.147389 -0.071566 0.000121  
H 4.599003 1.944280 0.000066 C 6.942046 -1.247543 0.000142 H 7.977692 -0.902173 0.000232 H  
6.768170 -1.858432 0.895261 H 6.768309 -1.858375 -0.895044

### 3.10 MC5

35

C 4.076673 -2.655892 0.006792 C 3.263543 -1.531318 0.003680 C 3.823415 -0.250196 -0.000111  
C 5.205225 -0.058712 -0.000891 C 6.010922 -1.202411 0.002272 C 5.464194 -2.486351 0.006069  
N 2.735778 0.691906 -0.002607 C 1.479384 0.057917 -0.000517 C 1.763923 -1.436524 0.003664 C  
0.237301 0.635057 -0.001870 C -0.928241 -0.178481 0.000708 C -2.250680 0.240078 -0.000160 C  
-2.664770 1.681751 -0.004123 C -4.110351 1.934627 -0.004700 C -5.025178 0.934973 -0.001643 C  
-4.588076 -0.435431 0.002248 C -3.267293 -0.770327 0.002953 O -1.855061 2.614299 -0.007234 N  
-5.590431 -1.495915 0.005482 O -6.776655 -1.156476 0.004936 N 2.931587 2.086840 -0.006780 O  
-5.201431 -2.667109 0.009022 H 3.638927 -3.650447 0.009740 H 6.115903 -3.354809 0.008467 H  
7.089498 -1.075921 0.001726 H 5.643501 0.926011 -0.003805 H 1.319976 -1.913624 0.886332 H  
1.319705 -1.918564 -0.876185 H 0.103755 1.703742 -0.004870 H -0.790419 -1.259363 0.003736 H  
-2.989741 -1.819273 0.005899 H -6.090862 1.131150 -0.002046 H -4.407559 2.978307 -0.007710 O  
4.095981 2.468680 -0.008227 O 1.934691 2.791653 -0.008563

## 4 Vertical excitations of SP1 with all the functionals



| method          | S <sub>1</sub> | S <sub>2</sub> | S <sub>3</sub> | S <sub>4</sub> | S <sub>5</sub> | score |
|-----------------|----------------|----------------|----------------|----------------|----------------|-------|
| ADC(2)          | 4.39 (0.04)    | 4.58 (0.04)    | 5.20 (0.13)    | 5.39(0.22)     | 5.76 (0.07)    |       |
| SPW92           | 3.05 (0.00)    | 3.87 (0.02)    | 3.93 (0.01)    | 4.09 (0.01)    | 4.23 (0.00)    | 0     |
| B97-D           | 3.13 (0.00)    | 3.94 (0.02)    | 4.02 (0.01)    | 4.15 (0.01)    | 4.28 (0.00)    | 0     |
| MPW91           | 3.10 (0.00)    | 3.91 (0.02)    | 3.99 (0.01)    | 4.13 (0.01)    | 4.25 (0.00)    | 0     |
| PBE             | 3.09 (0.00)    | 3.91 (0.02)    | 3.98 (0.01)    | 4.13 (0.01)    | 4.25 (0.00)    | 0     |
| BLYP            | 3.09 (0.00)    | 3.90 (0.02)    | 3.96 (0.01)    | 4.11 (0.01)    | 4.23 (0.00)    | 0     |
| N12             | 3.11 (0.00)    | 3.93 (0.02)    | 4.00 (0.01)    | 4.13 (0.01)    | 4.29 (0.00)    | 0     |
| B97M-V          | 3.43 (0.00)    | 4.24 (0.03)    | 4.38 (0.00)    | 4.47 (0.01)    | 4.62 (0.00)    | 14    |
| mBEEF           | 3.41 (0.00)    | 4.18 (0.03)    | 4.34 (0.00)    | 4.43 (0.01)    | 4.57 (0.00)    | 12    |
| M06-L           | 3.37 (0.00)    | 4.17 (0.03)    | 4.33 (0.00)    | 4.43 (0.01)    | 4.54 (0.00)    | 12    |
| revM06-L        | 3.62 (0.00)    | 4.44 (0.03)    | 4.66 (0.00)    | 4.75 (0.01)    | 4.88 (0.00)    | 23    |
| MN15-L          | 3.61 (0.00)    | 4.41 (0.03)    | 4.61 (0.00)    | 4.70 (0.01)    | 4.80 (0.00)    | 20    |
| revTPSS         | 3.26 (0.00)    | 4.06 (0.03)    | 4.18 (0.01)    | 4.32 (0.01)    | 4.41 (0.00)    | 6     |
| TPSS            | 3.22 (0.00)    | 4.03 (0.03)    | 4.13 (0.01)    | 4.27 (0.01)    | 4.37 (0.00)    | 5     |
| $\omega$ B97X-D | 4.65 (0.03)    | 4.97 (0.01)    | 5.04 (0.06)    | 5.26 (0.00)    | 5.86 (0.05)    | 63    |
| CAM-B3LYP       | 4.65 (0.02)    | 4.92 (0.03)    | 4.97 (0.03)    | 5.23 (0.01)    | 5.82 (0.05)    | 64    |
| $\omega$ B97X-V | 4.81 (0.03)    | 5.08 (0.01)    | 5.31 (0.04)    | 5.56 (0.05)    | 5.99 (0.02)    | 70    |
| SOGGA11-X       | 4.61 (0.00)    | 4.75 (0.05)    | 5.05 (0.01)    | 5.25 (0.01)    | 5.83 (0.05)    | 65    |
| LRC-wPBE        | 4.66 (0.03)    | 4.95 (0.01)    | 5.20 (0.07)    | 5.34 (0.01)    | 5.92 (0.05)    | 65    |
| LRC-wPBEh       | 4.63 (0.02)    | 4.95 (0.00)    | 4.99 (0.06)    | 5.25 (0.00)    | 5.86 (0.06)    | 60    |
| MPW1K           | 4.68 (0.01)    | 4.81 (0.05)    | 5.08 (0.01)    | 5.27 (0.01)    | 5.86 (0.05)    | 58    |
| PBE0            | 4.03 (0.01)    | 4.47 (0.04)    | 4.81 (0.01)    | 5.05 (0.01)    | 5.15 (0.01)    | 50    |
| HSEHJS          | 3.89 (0.01)    | 4.43 (0.04)    | 4.78 (0.01)    | 4.96 (0.00)    | 5.02 (0.01)    | 46    |
| rcamB3LYP       | 4.93 (0.04)    | 5.16 (0.01)    | 5.39 (0.03)    | 5.81 (0.08)    | 6.19 (0.01)    | 62    |
| MPW1PW91        | 4.68 (0.01)    | 4.81 (0.05)    | 5.08 (0.01)    | 5.27 (0.01)    | 5.86 (0.05)    | 58    |
| BHHLYP          | 4.81 (0.03)    | 5.02 (0.04)    | 5.14 (0.02)    | 5.31 (0.00)    | 5.87 (0.04)    | 63    |
| PBE50           | 4.83 (0.02)    | 5.03 (0.04)    | 5.17 (0.02)    | 5.35 (0.00)    | 5.93 (0.04)    | 63    |
| B3LYP           | 3.84 (0.01)    | 4.36 (0.04)    | 4.71 (0.01)    | 4.89 (0.00)    | 4.95 (0.01)    | 44    |
| HFLYP           | 5.26 (0.07)    | 5.64 (0.01)    | 5.69 (0.00)    | 5.98 (0.03)    | 6.88 (0.28)    | 23    |
| BMK             | 4.58 (0.01)    | 4.74 (0.05)    | 5.03 (0.01)    | 5.27 (0.01)    | 5.84 (0.03)    | 59    |
| M06-SX          | 4.25 (0.01)    | 4.62 (0.04)    | 5.00 (0.01)    | 5.19 (0.01)    | 5.41 (0.01)    | 55    |
| M06-2X          | 4.72 (0.02)    | 4.92 (0.04)    | 5.04 (0.02)    | 5.31 (0.01)    | 5.93 (0.07)    | 63    |
| $\omega$ B97M-V | 4.75 (0.03)    | 5.01 (0.01)    | 5.25 (0.04)    | 5.46 (0.04)    | 5.91 (0.03)    | 74    |
| wM05-D          | 4.10 (0.01)    | 4.41 (0.05)    | 4.76 (0.01)    | 4.95 (0.01)    | 5.22 (0.01)    | 47    |
| MN15            | 4.50 (0.01)    | 4.62 (0.05)    | 4.89 (0.01)    | 5.12 (0.01)    | 5.73 (0.05)    | 60    |
| PW6B95          | 4.08 (0.01)    | 4.47 (0.04)    | 4.80 (0.01)    | 5.05 (0.01)    | 5.21 (0.01)    | 51    |
| SCAN0           | 4.22 (0.01)    | 4.60 (0.04)    | 4.98 (0.01)    | 5.13 (0.01)    | 5.37 (0.01)    | 55    |
| M11             | 4.84 (0.03)    | 5.12 (0.01)    | 5.35 (0.05)    | 5.52 (0.03)    | 6.03 (0.04)    | 68    |
| revTPSSh        | 3.62 (0.01)    | 4.29 (0.04)    | 4.60 (0.00)    | 4.68 (0.00)    | 4.80 (0.01)    | 24    |
| TPSSh           | 3.58 (0.01)    | 4.26 (0.04)    | 4.56 (0.00)    | 4.65 (0.00)    | 4.76 (0.01)    | 24    |
| MN12SX          | 3.09 (0.00)    | 3.85 (0.03)    | 3.92 (0.01)    | 4.09 (0.00)    | 4.12 (0.01)    | 0     |

Table 2: energies, oscillator strengths (in parenthesis) for the first 5 vertical excitations of SP1 calculated with ADC(2)/def2-TZVP and TD-DFT/def2-TZVP with the 38 functionals selected. The calculated scores according to the developed scoring system are reported in the last column.

## **5 Vertical excitations of SP2 with all the functionals**

| method         | S <sub>1</sub> | S <sub>2</sub> | S <sub>3</sub> | S <sub>4</sub> | S <sub>5</sub> | score |
|----------------|----------------|----------------|----------------|----------------|----------------|-------|
| ADC(2)         | 3.87 (0.00)    | 4.39 (0.02)    | 4.44 (0.00)    | 4.55 (0.26)    | 4.60 (0.04)    |       |
| SPW92          | 2.12 (0.00)    | 2.88 (0.00)    | 3.10 (0.00)    | 3.25 (0.01)    | 3.45 (0.00)    | 0     |
| B97D           | 2.18 (0.00)    | 2.96 (0.00)    | 3.14 (0.00)    | 3.27 (0.01)    | 3.53 (0.00)    | 0     |
| MPW91          | 2.18 (0.00)    | 2.93 (0.00)    | 3.16 (0.00)    | 3.29 (0.01)    | 3.47 (0.00)    | 0     |
| PBE            | 2.19 (0.00)    | 2.92 (0.00)    | 3.18 (0.00)    | 3.30 (0.01)    | 3.47 (0.00)    | 0     |
| BLYP           | 2.14 (0.00)    | 2.92 (0.00)    | 3.10 (0.00)    | 3.24 (0.01)    | 3.46 (0.00)    | 0     |
| N12            | 2.07 (0.00)    | 2.92 (0.00)    | 3.02 (0.00)    | 3.17 (0.01)    | 3.52 (0.00)    | 0     |
| B97MV          | 2.46 (0.00)    | 3.25 (0.00)    | 3.44 (0.00)    | 3.54 (0.01)    | 3.83 (0.00)    | 0     |
| mBEEF          | 2.39 (0.00)    | 3.23 (0.00)    | 3.35 (0.00)    | 3.45 (0.01)    | 3.67 (0.00)    | 0     |
| M06L           | 2.45 (0.00)    | 3.20 (0.00)    | 3.44 (0.01)    | 3.53 (0.01)    | 3.69 (0.00)    | 0     |
| revM06L        | 2.67 (0.00)    | 3.44 (0.00)    | 3.69 (0.01)    | 3.78 (0.01)    | 3.87 (0.00)    | 1     |
| MN15L          | 2.71 (0.00)    | 3.44 (0.00)    | 3.71 (0.01)    | 3.79 (0.01)    | 4.03 (0.00)    | 0     |
| revTPSS        | 2.33 (0.00)    | 3.09 (0.00)    | 3.32 (0.00)    | 3.42 (0.01)    | 3.61 (0.00)    | 0     |
| TPSS           | 2.29 (0.00)    | 3.05 (0.00)    | 3.28 (0.00)    | 3.38 (0.01)    | 3.59 (0.00)    | 0     |
| $\omega$ B97XD | 3.95 (0.00)    | 4.47 (0.00)    | 4.47 (0.02)    | 4.61 (0.05)    | 4.88 (0.04)    | 43    |
| CAMB3LYP       | 3.95 (0.00)    | 4.41 (0.02)    | 4.48 (0.00)    | 4.52 (0.05)    | 4.73 (0.02)    | 49    |
| $\omega$ B97XV | 4.04 (0.00)    | 4.56 (0.00)    | 4.72 (0.03)    | 4.79 (0.05)    | 5.10 (0.01)    | 56    |
| SOGGA11X       | 4.13 (0.00)    | 4.16 (0.01)    | 4.38 (0.04)    | 4.57 (0.01)    | 4.65 (0.00)    | 18    |
| LRCwPBE        | 3.86 (0.00)    | 4.40 (0.00)    | 4.56 (0.02)    | 4.69 (0.07)    | 4.97 (0.01)    | 44    |
| LRCwPBEh       | 3.93 (0.00)    | 4.46 (0.02)    | 4.46 (0.00)    | 4.60 (0.06)    | 4.83 (0.04)    | 51    |
| MPW1K          | 4.13 (0.00)    | 4.25 (0.01)    | 4.42 (0.04)    | 4.62 (0.00)    | 4.66 (0.01)    | 23    |
| PBE0           | 3.39 (0.00)    | 3.88 (0.00)    | 3.89 (0.00)    | 3.99 (0.03)    | 4.39 (0.02)    | 24    |
| HSEHJS         | 3.11 (0.00)    | 3.73 (0.01)    | 3.87 (0.00)    | 3.91 (0.03)    | 4.17 (0.00)    | 13    |
| rcamB3LYP      | 4.09 (0.00)    | 4.61 (0.00)    | 4.86 (0.02)    | 4.89 (0.05)    | 5.18 (0.02)    | 49    |
| BHHLYP         | 4.23 (0.00)    | 4.50 (0.01)    | 4.56 (0.05)    | 4.71 (0.00)    | 4.81 (0.01)    | 30    |
| PBE50          | 4.24 (0.00)    | 4.54 (0.00)    | 4.60 (0.06)    | 4.71 (0.00)    | 4.84 (0.02)    | 29    |
| BMK            | 3.96 (0.00)    | 4.12 (0.01)    | 4.37 (0.04)    | 4.47 (0.00)    | 4.52 (0.01)    | 24    |
| M06SX          | 3.55 (0.00)    | 3.93 (0.00)    | 4.10 (0.00)    | 4.17 (0.04)    | 4.44 (0.00)    | 24    |
| M062X          | 4.08 (0.00)    | 4.50 (0.00)    | 4.55 (0.00)    | 4.58 (0.07)    | 4.78 (0.02)    | 41    |
| $\omega$ B97MV | 4.03 (0.00)    | 4.54 (0.00)    | 4.67 (0.02)    | 4.75 (0.05)    | 5.04 (0.01)    | 57    |
| wM05D          | 3.47 (0.00)    | 3.74 (0.00)    | 3.93 (0.02)    | 4.00 (0.02)    | 4.22 (0.00)    | 13    |
| MN15           | 3.87 (0.00)    | 4.10 (0.01)    | 4.28 (0.04)    | 4.37 (0.00)    | 4.47 (0.01)    | 29    |
| PW6B95         | 3.48 (0.00)    | 3.87 (0.00)    | 3.95 (0.00)    | 4.02 (0.03)    | 4.38 (0.00)    | 17    |
| SCAN0          | 3.55 (0.00)    | 4.06 (0.00)    | 4.07 (0.00)    | 4.12 (0.03)    | 4.52 (0.02)    | 26    |
| M11            | 4.02 (0.00)    | 4.48 (0.00)    | 4.75 (0.03)    | 4.83 (0.05)    | 5.15 (0.01)    | 49    |
| revTPSSh       | 2.79 (0.00)    | 3.46 (0.00)    | 3.67 (0.02)    | 3.78 (0.00)    | 3.86 (0.00)    | 3     |
| TPSSh          | 2.76 (0.00)    | 3.42 (0.00)    | 3.65 (0.02)    | 3.76 (0.00)    | 3.82 (0.00)    | 2     |
| MN12SX         | 2.59 (0.00)    | 2.97 (0.00)    | 3.46 (0.00)    | 3.58 (0.01)    | 3.67 (0.00)    | 2     |
| B3LYP          | 3.10 (0.00)    | 3.69 (0.00)    | 3.79 (0.01)    | 3.80 (0.02)    | 4.15 (0.00)    | 7     |
| HFLYP          | 5.07 (0.00)    | 5.16 (0.02)    | 5.38 (0.00)    | 5.40 (0.03)    | 5.66 (0.03)    | 32    |

Table 3: energies, oscillator strengths (in parenthesis) for the first 5 vertical excitations of SP2 calculated with ADC(2)/def2-TZVP and TD-DFT/def2-TZVP with the 38 functionals selected. The calculated scores according to the developed scoring system are reported in the last column.

## 6 OPV XYZ coordinates optimized at B3LYP/def2-SVP level used for the in-silico experiment

### 6.1 OPV1

60

C -26.07722499318305 10.89855897233370 0.88125015250551 N -25.01682242343919 11.64192786105441  
0.19994323239472 C -23.71071444141026 11.15316782984565 0.24184241951866 O -23.44509443096064  
10.12899578035277 0.84313964098150 C -22.68299193932413 11.95834152499953 -0.48570463345798  
C -21.41995125008697 11.43372625684109 -0.42385814084842 C -20.12756508213729 11.80729297003905  
-0.89921018922455 O -19.86464318648718 12.94266463924378 -1.59954437115061 C -18.55124237584207  
12.98636367547647 -1.86770141502874 C -17.90729063653653 11.89699211440266 -1.33868505855433  
C -18.92010919133022 11.11949820641972 -0.70160150086527 C -18.76903880433972 9.80885361701719  
-0.01012966346992 O -19.66339492350663 8.97446564973312 -0.03164110727871 C -17.51057489177238  
9.54109886232953 0.70748098158117 C -16.49317829012580 10.39699824694412 1.11289552412075  
C -15.48417672892692 9.73498577751688 1.84742542682297 C -15.74345497484322 8.38103289130971  
1.99680125794208 C -14.92484816770309 7.39169263262504 2.69547499958544 N -13.77316032916372  
7.80939105083003 3.24471962321465 C -13.04070550973568 6.90896540409680 3.88910374058136  
C -13.43257497631724 5.55861765816502 4.01737446640463 C -12.68479322725203 4.54208398130534  
4.77580516384815 C -13.32149137462557 3.63792314519464 5.56362174517856 C -12.60801819179173  
2.55446391503125 6.23549737236858 C -11.26684457020191 2.57714212790917 6.34575096907069  
C -10.51737180991803 3.76982626293569 5.81786173527050 N -9.09923198446563 3.49595745713567  
5.59133022340069 C -8.51352423421778 4.29059850679275 4.81636773226856 F -7.21973306644321  
4.17299504851034 4.54809503644493 C -9.21633338558188 5.41715544226497 4.13969799559700  
F -8.44066928907728 6.38508063625117 3.67161118210522 N -10.46632242945664 5.47320842260050  
4.03509114447609 C -11.19163727452563 4.32161360850599 4.55921679106768 C -14.64910186447748  
5.23841171319152 3.38326448499065 N -15.38720565304215 6.13238426870478 2.73855288217300  
S -17.23516931522274 7.91029134780274 1.25118071654381 C -23.06962907241834 13.19999412362597  
-1.19210989383941 O -22.30014061550325 13.89552700775935 -1.82434906703008 N -24.42613108168455  
13.55169286156059 -1.09320766488068 C -24.88327876623171 14.77473804506479 -1.75275702035908  
C -25.41094747472798 12.81779278338754 -0.43694746597275 O -26.56738076079135 13.18605460837579  
-0.41855301093843 H -25.62639683107370 9.99789763173428 1.30863812975776 H -26.86867074346260  
10.63446648385714 0.16622984000841 H -26.52501142161436 11.51646278165313 1.67268209116087  
H -21.37983283704099 10.48445577086627 0.11986500392682 H -18.20971234895018 13.84088783576638  
-2.44720917538438 H -16.85107731587562 11.65896045994163 -1.42696310578746 H -16.49615245055915  
11.46789769224717 0.91289478487299 H -14.59506465228598 10.20261918980740 2.26929174623620

H -12.10687396830243 7.25717721020180 4.33500675530701 H -14.40398966243878 3.70597402093461  
5.69740113971492 H -13.18942101019044 1.74155820166218 6.67780999068572 H -10.69897846039415  
1.80854949036873 6.87438775494136 H -10.56456660514723 4.56256821496265 6.60133628949623  
H -11.12489291193431 3.53017044588317 3.77734964992979 H -15.01704669134990 4.20568007804239  
3.39316903654274 H -24.00194772542042 15.28201573278037 -2.15613550120190 H -25.40697320553370  
15.41530090971472 -1.03034628675557 H -25.58524816959565 14.53252091408837 -2.56436458101028

## 6.2 OPV2

60

C -4.25286603107688 -6.69455136074366 3.60324534312832 N -3.15582413608782 -6.19143365563910  
2.77576830416281 C -2.26059302809397 -5.27022918568120 3.32109035484426 O -2.35450998338002  
-4.90310274258316 4.47842005536237 C -1.23599843717346 -4.74334257950764 2.37963303907623  
C -0.49330155958890 -3.69395900026078 2.83770690555358 C 0.45284545621465 -2.82059196343638  
2.18564848447269 C 1.44519305120770 -2.25177264248344 2.93523997100478 C 2.50245984662958  
-1.46256613347051 2.34998423982888 C 2.40570948329348 -0.94978236712274 1.09173447698126  
C 3.46606281344246 -0.10304628429610 0.53155208209417 C 4.15591838968894 0.82379837628977  
1.34142396539178 N 5.17228228136116 1.55470348450637 0.90809549722338 C 5.53989238204274  
1.38851483801690 -0.37407251844722 C 6.67740025341006 2.16450077305407 -0.85698585195198  
C 7.42637696780625 3.08709101769498 -0.14246919309978 C 8.47603900201288 3.63828471661067  
-0.91131952574076 C 8.51754610656420 3.13148921042583 -2.20362520751124 C 9.39703971994498  
3.45929002890836 -3.34577278489158 O 9.07923994321974 3.13107511161665 -4.48076702645161  
C 10.65910522011074 4.19574029323021 -3.09759264345940 C 11.47648920244801 4.33973665446749  
-1.91524779205525 C 12.55005702498337 5.09206872034236 -2.28901897024786 O 12.45581911126728  
5.42685396279837 -3.60699084713663 C 11.32613316667185 4.87660285550694 -4.08871706977617  
S 7.24300052748904 1.98150089968085 -2.48603472376528 N 4.93962949465961 0.55841999045825  
-1.24368586633162 C 3.92065901088025 -0.16829666766307 -0.80430389145492 C 1.06956239014565  
-1.15137866384655 0.39846030986715 N 1.08113355302535 -0.89937140980042 -1.03719311127038  
C 0.07165210029081 -1.30592729671252 -1.66423959044315 F -0.05608946454187 -1.11320791742757  
-2.96812692433600 C -1.03395493706479 -2.04462918621642 -0.99605963273747 F -2.19369794619505  
-2.06800955706715 -1.64117757572226 N -0.89160467329952 -2.59675560223260 0.12054874306311  
C 0.45083380488113 -2.52389013928515 0.69892433326755 C -1.01500317103061 -5.41105612965942  
1.08202171943228 O -0.01098476286733 -5.26056476319438 0.40593704956539 N -2.02816039877094  
-6.27950362247951 0.67416648882333 C -1.93593794346427 -6.91057651210458 -0.64243515600770  
C -3.10227746254977 -6.68285244774097 1.47004619349576 O -3.93642680873690 -7.45899654985022  
1.05527254604276 H -4.17991423657560 -6.20550571083842 4.57931186745861 H -4.17469452351787

-7.78541912091392 3.71469349034142 H -5.21671508678284 -6.46821852159758 3.12684134115349  
H -0.67008478224239 -3.47087627899276 3.89635700716998 H 1.49789354755191 -2.47746412218780  
4.00385061998509 H 3.40128275784308 -1.28292887058877 2.94389881000895 H 3.84094309385844  
0.98236926891728 2.37976046405694 H 7.19978727682522 3.33719726231886 0.89354572312033  
H 9.15794559293580 4.40496187568516 -0.54661102295847 H 11.30709883377441 3.90442151107550  
-0.93462994932718 H 13.43166470560653 5.45210323485269 -1.76550476147275 H 11.09561711690350  
5.03931785260850 -5.13786630974625 H 3.44570161009932 -0.84245394340664 -1.51944278498678  
H 0.39806775591757 -0.38368990967665 0.84715521317642 H 1.05347387317169 -3.30903383518654  
0.20428080455117 H -1.09945755490783 -6.44709783102320 -1.17374742370115 H -2.87787819049973  
-6.76521906797481 -1.18710546704455 H -1.76088134973136 -7.99210034617363 -0.54154182162889

### 6.3 OPV3

55

C -2.85298952981912 -0.71730199672566 -2.24744821004828 N -1.68651532449737 -1.57652529484767  
-2.03396895476738 C -0.96005670936472 -1.44907715180233 -0.85249385235672 O -1.27667029097863  
-0.65970953291526 0.01480756580850 C 0.25094974661205 -2.31715215461263 -0.75378307494016  
C 1.07691586391843 -2.09940981478011 0.29102783894502 C 2.38386052083998 -2.74064933151631  
0.53173625531416 N 3.31381602446010 -2.71458004818288 -0.43776340234298 C 4.44920215688240  
-3.31723572135018 -0.15745800983388 C 4.63772984389320 -3.96691719468899 1.08632462678232  
C 5.84150625897180 -4.71457383412291 1.43405679789400 C 6.08068352415705 -5.36044968238116  
2.63737770845823 C 7.33820577047237 -6.00623596330913 2.66677978730728 C 8.05271116801927  
-5.85428586014319 1.48823623634613 C 9.40924580998898 -6.29710622899343 1.09838172784875  
O 9.97382224793004 -5.77060431759359 0.14994168688137 C 10.04659536706778 -7.38694778690801  
1.87151536907592 C 9.42584420930374 -8.40902996555539 2.54760096796528 O 10.33938489511500  
-9.25893959935790 3.05924592743764 C 11.57133751977953 -8.79383480713577 2.72821167891417  
C 11.47671762437908 -7.64221778134941 1.98406739440088 C 12.55066700994591 -6.83085418804086  
1.42976484270740 C 13.85995412575572 -6.96395682846562 1.73099675234322 C 14.90622334937703  
-6.13124824480202 1.13510476924876 C 16.25901369682753 -6.30743538595382 1.47832800105783  
C 17.18872043983341 -5.47001912068674 0.86425746076164 N 16.83420642445821 -4.53149401688704  
-0.01713819090487 C 15.52421858837530 -4.44217432018162 -0.27617712056157 N 14.55395087785073  
-5.18237510155019 0.24595189614102 S 7.17946839971506 -4.88685678179105 0.33629996284802  
N 3.68202243795091 -3.88301571613207 2.02610396351586 N 2.56251873255828 -3.24503521773613  
1.75779253275564 C 0.48514134367905 -3.40510133088987 -1.74212059319014 O 1.30004405875851  
-4.29080713612134 -1.57840826541737 N -0.32324525873222 -3.35500127929435 -2.87779359026320  
C -0.11955156370206 -4.34543736112443 -3.93677555703601 C -1.39276717518571 -2.47416793450881

-3.06548632400798 O -2.05963311775596 -2.50512819575001 -4.07635499323678 H -2.94564249243930  
-0.06552058910319 -1.37345576681580 H -3.75719390856353 -1.33075132621322 -2.36595884448026  
H -2.71897604457264 -0.12312150626671 -3.16170379339991 H 0.74075693874639 -1.37106387809127  
1.03673052153584 H 5.24271160299418 -3.29291469168767 -0.91429920563385 H 5.35818435360425  
-5.34304517961565 3.45253255690297 H 7.72968727630576 -6.53485490456870 3.53495427297318  
H 8.38304109430368 -8.67325499078968 2.69730986734984 H 12.41334482141560 -9.38782414475761  
3.07245924834188 H 12.26129671549734 -6.05994270482577 0.71289642157079 H 14.19863802296201  
-7.71251608718022 2.45444552592589 H 16.56717053970828 -7.06977497221582 2.19715258991651  
H 18.25801717785480 -5.55952551654342 1.09164292561690 H 15.21975383426881 -3.67393241142630  
-0.99821860621965 H 0.76722896221494 -4.93094299119817 -3.67586851771323 H 0.01672227199893  
-3.83593403837752 -4.89981864189604 H -0.99637023314050 -5.00419783895095 -4.01729216582681

#### 6.4 OPV4

55

C 7.06857256803383 -9.38132344697572 -1.39795649547578 N 6.39092145314342 -8.35019101596139  
-0.60918359581239 C 5.52070835126982 -7.46719466050216 -1.24351858572463 O 5.33599066480546  
-7.50772470126374 -2.44576520248761 C 4.88283956003823 -6.44871141623017 -0.35776719302087  
C 4.26513057040867 -5.41640633071627 -0.97754403978692 C 3.65327261708354 -4.21848680646603  
-0.36421084567389 N 2.52908668358814 -3.76778572292752 -0.94045078491619 C 1.96580863567441  
-2.70159562024945 -0.36680003700586 C 2.51211908756372 -2.07089587525756 0.75148424118685  
C 3.71599239798219 -2.59445992352527 1.25774783648699 C 4.42133643163125 -2.03519331299283  
2.41894705216087 C 5.41580423529599 -2.75075569549434 2.98294112687852 C 6.34201740584104  
-2.38467133986485 4.03937579651327 C 6.20198814625725 -1.50655145794706 5.08610130307002  
O 7.30775342426258 -1.52287451859613 5.87273213782668 C 8.17616091227970 -2.41886491070727  
5.35405698717397 C 7.65945746552674 -2.98163126820915 4.21781708652655 C 8.33285912585886  
-4.02536852865490 3.39524171761118 O 8.97324390490037 -4.92983548183668 3.91096587517187  
C 8.16814773396961 -3.93935542387815 1.93129635496513 C 7.73767688274953 -2.88601143063294  
1.14092225073387 C 7.61590779286764 -3.22905265839175 -0.22333227098162 C 7.97914874268864  
-4.54084775572432 -0.47571468373207 C 7.91311211768649 -5.21396257402608 -1.77004614120818  
C 8.60223574751562 -6.40802692615006 -2.06773643131808 N 8.46045559119193 -6.99210004926380  
-3.24510401404063 C 7.65294472100728 -6.36396181819629 -4.10720744969250 N 7.02693423748180  
-5.20488337431263 -3.89096392303550 N 7.14878758196227 -4.63255848491726 -2.71107051905502  
S 8.48797492913751 -5.35810465325648 0.97316430954479 N 4.27648501416731 -3.65925335921153  
0.66585328968314 C 4.93335592974247 -6.62905121165736 1.12098712959766 O 4.17575775196825  
-6.09014274785931 1.89980202309697 N 5.94537718209533 -7.48478620182609 1.57166580592728

C 6.23676932077044 -7.54686958628561 3.00508110032351 C 6.69619889238116 -8.32906401809251  
0.75856940355919 O 7.55615916536007 -9.05088827957336 1.21440632958648 H 6.79794239398901  
-9.23074387780443 -2.44620555795823 H 6.75533823941678 -10.37894438212355 -1.05728308072328  
H 8.15542140704943 -9.30074978934893 -1.27280295471922 H 4.21990842443450 -5.46543799262914  
-2.06982362939690 H 1.04039297762831 -2.32897439429922 -0.82111248941876 H 2.02700235336019  
-1.20719454004948 1.21070034415289 H 4.13842045834052 -1.03694045300649 2.76611021526513  
H 5.58143047391427 -3.73175894296092 2.53472043157569 H 5.38608554979538 -0.86735762101698  
5.41271540922601 H 9.12397116413972 -2.54580766351353 5.87021697859602 H 7.50503437224285  
-1.90223125428314 1.54412496897667 H 7.26555040390505 -2.56593803291533 -1.01284481801943  
H 9.27227791113049 -6.87497778817167 -1.33511567517558 H 7.48837545391418 -6.82390441539381  
-5.08626011391331 H 5.48150247985580 -6.94598691615525 3.52052980204462 H 7.24320397208593  
-7.14812843920341 3.20331025240446 H 6.20063898860853 -8.58755090949032 3.35275297242609

## 6.5 OPV5

53

C -2.07665862815402 0.01546881581173 -1.71341197317336 N -0.65765547328186 -0.25576480860913  
-1.47680444825034 C -0.25883825674602 -0.73800964564156 -0.23519757379069 O -1.04310735421148  
-0.90378513702795 0.67927197972584 C 1.18813045003266 -1.09155217230969 -0.13502694314401  
C 1.54984417611516 -1.84260055746575 0.93375234891753 C 2.81672258726890 -2.49801250300038  
1.19313921458215 S 3.39358061916191 -2.59168795925478 2.82442226842640 C 4.77533813214251  
-3.53298448668388 2.34711647518763 C 5.70266740059190 -3.90474147215049 3.35490334666410  
N 6.38348068172492 -4.14381013076436 4.26612813489259 C 4.78320655808265 -3.79380313806387  
0.97840138698091 C 5.82906844170929 -4.57607882052042 0.29676899351084 N 6.79168762504625  
-5.11265627945648 1.05104813788407 C 7.74367993831965 -5.79826200940234 0.42657786102257  
C 7.76137647246405 -5.97112841822022 -0.96696030564430 C 8.80847888295878 -6.76323553671254  
-1.63428737445755 C 9.25459462938764 -8.02041050394480 -1.11894148656620 C 10.22486273401436  
-8.60731287288175 -1.89322765266446 S 10.61407351962069 -7.65353984337874 -3.26971153536594  
C 9.46024565375956 -6.42211886174774 -2.82003616360678 C 9.38274092617995 -5.12055243482930  
-3.53577770511246 O 8.98069677068092 -4.12433144292080 -2.95187616902999 C 9.80983813499889  
-5.03708436664753 -4.95045013964590 C 9.98387478406766 -6.04431621708528 -5.97286316232329  
C 10.34764140283460 -5.37336889115680 -7.10177032492283 O 10.41542587437773 -4.03372636834067  
-6.85414572558493 C 10.08372819180608 -3.83739471264469 -5.56734296380778 C 6.68461308442223  
-5.38099272665002 -1.65455108993488 N 5.73851595706510 -4.69313543716162 -1.03329536944058  
C 3.65227440636344 -3.20241638972108 0.32198931509751 C 3.30033495029167 -3.35499326156411  
-1.05446165628147 N 2.86905759053993 -3.41507949275575 -2.13083919873876 C 2.14664061922642



-0.57106313584004 -1.14582024939964 O 3.34041497915069 -0.48320712697206 -0.94584978021822  
N 1.56896942867922 -0.18133277468812 -2.35071497523138 C 2.44040487807137 0.15284216039875  
-3.47834825521389 C 0.19772814557013 -0.03460285934585 -2.56554515469252 O -0.23889474259409  
0.31429965998302 -3.63963357404519 H -2.61328852765734 -0.20284802560775 -0.78505906734981  
H -2.44870452400031 -0.61607160356954 -2.53201269870233 H -2.21710757832163 1.06697845740920  
-2.00025705638271 H 0.75440869990338 -2.00213080327482 1.67164458199220 H 8.53955108261965  
-6.21993167544995 1.05121313024945 H 8.84841850990437 -8.47634973708651 -0.21506378878914  
H 10.72723921885008 -9.55950422330932 -1.72648389765910 H 9.82879034465781 -7.11589277570544  
-5.88490777730518 H 10.57507914574082 -5.68443013987880 -8.11775179539253 H 10.08093992334408  
-2.81575628874737 -5.19749352809292 H 6.58994717310112 -5.48532703085687 -2.73982855670813  
H 3.46955517306533 -0.05492979042503 -3.17084879059883 H 2.33049151257613 1.21305283798693  
-3.74814243825105 H 2.16534567447674 -0.46035704211742 -4.34628682961456

## 7 Supplementary links

- Repository containing the results of the calculations, collected in energies and oscillator strengths (extended-QM8) and overlap matrices between TD-DFT functionals and ADC(2) reference:  
<https://figshare.com/projects/DELFI/185308>
- GitHub repository containing model parameters, the training data, the code to calculate the scoring system and to launch the web application:  
<https://github.com/aspuru-guzik-group/DELFI>
- Web application:  
<https://delfi-functional-predictor.streamlit.app/>