Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supplementary Information

Open-shell donor$-\pi-$acceptor conjugated metal-free dyes for dye-sensitized solar cells

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Table S1: Calculated diradical index (y) of the open-shell (MS3–MS8) dyes in their ground-state at different functional and 6-31G(d, p) basis set. Calculations with UCAM-B3LYP and UBHandLYP are performed on UB3LYP optimized geometry.

Dyes	UB3LYP	UCAM-B3LYP	UBHandLYP
MS3	0.096	0.429	0.530
MS4	0.086	0.414	0.517
MS5	0.065	0.401	0.510
MS6	0.130	0.452	0.550
MS7	0.123	0.443	0.542
MS8	0.115	0.444	0.547

Table S2: Spin-squared $< S^2 >$ values of the open-shell (MS3–MS8) dyes in their ground-state at different functional and 6-31G(d, p) basis set. Calculations with UCAM-B3LYP and UBHandLYP are performed on UB3LYP optimized geometry.

Dyes	UB3LYP	UCAM-B3LYP	UBHandLYP
MS3	0.00951	0.620737	1.775334
MS4	0.007852	0.574221	1.676901
MS5	0.00436	0.76172	1.680451
MS6	0.018026	0.743505	2.067553
MS7	0.016094	0.704464	1.983108
MS8	0.01491	0. 734786	2.169022

Table S3: Cartesian coordinates of D35 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(d, p) basis set.

Atom symbol	X	Y	Z
C	1.25800000	-1.26703600	0.06915700
C	0.77134500	-2.30430700	-0.74013200
C	2.29662600	-1.54493900	0.96700800
C	1.29877500	-3.58696000	-0.64017900
H	-0.02765800	-2.10086500	-1.44575600
C	2.83032300	-2.82748000	1.04739500
H	2.69143300	-0.74989100	1.59092400
C	2.34212200	-3.88175200	0.25570500
H	0.90418500	-4.37175900	-1.27404400
H	3.65007800	-3.01425900	1.73445500

C	1.63380000	1.15125800	-0.11552000
C	1.45893200	2.29076900	0.68369100
C	2.73381900	1.09908300	-0.98119000
C	2.35114300	3.35432100	0.60494900
H	0.61557200	2.34075900	1.36483700
C	3.63135400	2.16076000	-1.04023700
H	2.88875800	0.21911100	-1.59672000
C	3.46064300	3.31682200	-0.25858500
H	2.19320600	4.22439900	1.23061000
H	4.48911100	2.08849700	-1.70201600
C	-0.66163400	0.26728900	-0.05377900
C	-1.54170500	-0.60488000	0.61911900
C	-1.21855900	1.36082100	-0.74879100
C	-2.91016200	-0.38965500	0.59388100
H	-1.14051400	-1.44409100	1.17516000
C	-2.58788900	1.56971000	-0.76377500
H	-0.56706800	2.03576100	-1.29152600
C	-3.47517100	0.70277400	-0.09356500
H	-3.55309900	-1.06558600	1.15064500
H	-2.98156100	2.40162800	-1.33888800
C	-4.91221500	0.94164300	-0.11988900
C	-5.58077100	2.12757400	-0.40848800
S	-6.06201300	-0.32248900	0.22356500
C	-6.97936300	2.03100200	-0.34587100
C	-7.43514300	0.75967900	-0.00480200
H	-7.64651000	2.86323300	-0.52915600
C	-8.74704200	0.23597800	0.17334000

H	-8.82373000	-0.81138000	0.45904100
C	-9.96577300	0.85151600	0.03800500
C	-10.11884200	2.21897200	-0.32871100
C	-11.17502900	0.03075600	0.29219200
N	-10.20834100	3.34125000	-0.62995800
O	-11.16399700	-1.14329500	0.61019900
O	-12.31831200	0.73531400	0.13114100
H	-13.04337100	0.11643700	0.31779700
H	-5.06099300	3.05201900	-0.62874800
N	0.72567400	0.05325200	-0.03396700
C	4.40632900	4.45394400	-0.39576900
C	4.91422800	5.17542500	0.70845800
C	4.85417800	4.84487500	-1.66811400
C	5.82073400	6.22963300	0.53287800
C	5.75126900	5.88588400	-1.86467100
H	4.46239600	4.32001000	-2.53398500
C	6.23819100	6.58398600	-0.75568700
H	6.19955600	6.76277500	1.39245600
H	6.07565000	6.17798700	-2.85692900
C	2.89644000	-5.25046500	0.41548100
C	3.19493100	-6.09671900	-0.67656500
C	3.16797700	-5.75242500	1.69866000
C	3.73535700	-7.37457000	-0.47917400
C	3.70279100	-7.01476700	1.91679800
H	2.92758500	-5.12983300	2.55498300
C	3.98843800	-7.83243900	0.81948900
H	3.96052000	-8.00114500	-1.32965300

H	3.89459300	-7.38660000	2.91683500
O	7.11255200	7.59738300	-1.02280300
O	4.48842100	4.77649500	1.94518700
O	4.50785100	-9.06127900	1.10763800
O	2.94573400	-5.59363400	-1.92346200
C	7.63728600	8.34630600	0.06105500
H	8.29945700	9.09205200	-0.38100200
H	6.84492800	8.85753000	0.62300000
H	8.21542900	7.71557600	0.74876800
C	5.01569300	5.41465800	3.09632600
H	6.10580700	5.30438000	3.15737100
H	4.75988000	6.48169100	3.12471800
H	4.55696600	4.91509100	3.95078400
C	3.28742000	-6.36734700	-3.06144100
H	4.36116200	-6.59191900	-3.09141300
H	2.72203500	-7.30734800	-3.10060900
H	3.02509400	-5.75704700	-3.92678200
C	4.81329100	-9.93876200	0.03633800
H	5.20608500	-10.84760500	0.49431800
H	3.92030700	-10.18942200	-0.55078700
H	5.57477700	-9.51534100	-0.63140100

Table S4: Cartesian coordinates of MS1 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(d, p) basis set.

Atom symbol	X	Y	Z
C	-2.44049000	-1.16288800	-0.12147100
C	-2.17176600	-2.27433000	0.69051100

C	-3.54675100	-1.20344800	-0.97927300
C	-2.98067100	-3.40352000	0.63136700
H	-1.32260900	-2.25010800	1.36564800
C	-4.35880500	-2.33216900	-1.02077900
H	-3.77258700	-0.34489200	-1.60298300
C	-4.09446000	-3.46186900	-0.22589200
H	-2.75289300	-4.25084800	1.26629900
H	-5.22356200	-2.33459300	-1.67714800
C	-2.26629900	1.27542900	0.05893000
C	-1.90305500	2.34367500	-0.77393600
C	-3.29562000	1.46294200	0.98979400
C	-2.54301200	3.57303700	-0.66435300
H	-1.11283000	2.20680300	-1.50488300
C	-3.94002000	2.69234400	1.08191800
H	-3.59433300	0.64036600	1.63111100
C	-3.57731600	3.77932500	0.26652700
H	-2.24421300	4.38454800	-1.31637400
H	-4.74950500	2.81010400	1.79568600
C	-0.22876100	-0.09019500	-0.10277700
C	0.40744700	-1.17064700	-0.75410100
C	0.59109200	0.88977300	0.50050800
C	1.78497600	-1.26836700	-0.78891000
H	-0.19360000	-1.92341900	-1.25027300
C	1.96786800	0.79697800	0.44327600
H	0.13331800	1.71517800	1.03266800
C	2.61933000	-0.28669900	-0.19800000
H	2.23365400	-2.10275500	-1.31004100

H	2.56006900	1.55836900	0.93232100
C	4.07026200	-0.38322800	-0.23843600
C	4.78034900	-1.62450300	-0.29669800
C	4.93074900	0.76003000	-0.23594500
C	6.24644300	-1.70732800	-0.28863600
N	4.19717500	-2.83979500	-0.32109300
C	6.39928000	0.67136900	-0.22999700
N	4.49425600	2.03338000	-0.31373100
C	7.09501000	-0.56718200	-0.20615500
N	6.70095000	-2.97369500	-0.31835100
S	5.39116000	-3.94706600	-0.35507300
N	6.99500900	1.87172000	-0.32568200
S	5.81122300	2.98970800	-0.37867500
C	8.51541800	-0.75757300	-0.16797300
H	8.86107700	-1.70256600	-0.58125000
C	9.52104400	0.01719400	0.34540500
C	9.34507800	1.17817100	1.15627800
C	10.91001800	-0.48705400	0.14977700
N	9.23668100	2.08612400	1.87729700
O	11.20475700	-1.49130700	-0.46902700
O	11.83563600	0.30349900	0.73867900
H	12.69488000	-0.10873400	0.55078000
N	-1.62104200	0.00574300	-0.05656400
C	-4.24892400	5.09248700	0.43732800
C	-4.65407500	5.90169200	-0.64865100
C	-4.52734400	5.57535300	1.72663800
C	-5.30200200	7.12643900	-0.43945800

C	-5.16683000	6.78551200	1.95608400
H	-4.20620200	4.98289800	2.57780500
C	-5.55719100	7.56751600	0.86464700
H	-5.60768200	7.72501600	-1.28491100
H	-5.36144300	7.14505600	2.96001300
C	-4.95062900	-4.66933100	-0.34299900
C	-5.38847300	-5.41879000	0.77280100
C	-5.38043700	-5.10447200	-1.60745700
C	-6.21166600	-6.54182400	0.61534500
C	-6.19478400	-6.21407100	-1.78576000
H	-5.03988400	-4.55858900	-2.48191600
C	-6.61365300	-6.93878200	-0.66573300
H	-6.53851900	-7.09552700	1.48316600
H	-6.50555400	-6.53946500	-2.77195300
O	-6.17639000	8.74557400	1.16389000
O	-4.39729400	5.41554600	-1.90036300
O	-7.40818700	-8.01921400	-0.91524600
O	-4.98249500	-4.97717500	2.00121400
C	-6.58819900	9.58799000	0.09959200
H	-7.04657700	10.46059100	0.56685000
H	-5.73745400	9.91347500	-0.51281400
H	-7.32782300	9.09580400	-0.54507000
C	-4.83865300	6.14941700	-3.03091400
H	-5.92856000	6.27655900	-3.03092700
H	-4.36088200	7.13580000	-3.08868200
H	-4.54688000	5.56009900	-3.90129900
C	-5.44526200	-5.64517300	3.16366200

H	-6.53984300	-5.61994800	3.23638200
H	-5.10593000	-6.68840300	3.19677600
H	-5.01758800	-5.10385000	4.00866600
C	-7.86012600	-8.79945900	0.17973300
H	-8.46569300	-9.59851200	-0.25001100
H	-7.02341300	-9.24183600	0.73559500
H	-8.47900800	-8.21123500	0.86953300

Table S5: Cartesian coordinates of MS2 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*
C	-2.41901400	-1.15230500	-0.13449300
C	-2.15669000	-2.26639400	0.67577700
C	-3.51117500	-1.19641300	-1.00960600
C	-2.95634000	-3.40131300	0.59759700
H	-1.31877500	-2.24009500	1.36499400
C	-4.31607800	-2.32992000	-1.06892300
H	-3.73324600	-0.33568500	-1.63179100
C	-4.05643900	-3.46221000	-0.27672600
H	-2.73280500	-4.25074700	1.23140000
H	-5.17095400	-2.33418100	-1.73819500
C	-2.26141900	1.28622300	0.07451100
C	-1.90629000	2.36446100	-0.74870800
C	-3.29171400	1.45903700	1.00681200
C	-2.55392100	3.58898700	-0.62744300
H	-1.11463800	2.24078600	-1.48062000
C	-3.94605600	2.68276300	1.10884500

H	-3.58512200	0.62860600	1.64053900
C	-3.59034900	3.77954600	0.30413100
H	-2.25937300	4.40869300	-1.27118200
H	-4.75716300	2.78813700	1.82280700
C	-0.21255900	-0.06628500	-0.09607700
C	0.42840800	-1.13344200	-0.76027600
C	0.60028400	0.91138900	0.51798000
C	1.81055000	-1.22149000	-0.78906500
H	-0.16654100	-1.88187200	-1.26984300
C	1.98057400	0.82673700	0.46429400
H	0.13698600	1.73381700	1.04971000
C	2.62865800	-0.24789700	-0.17987800
H	2.26141600	-2.03116500	-1.35363600
H	2.57124700	1.58955700	0.95641700
C	4.09179500	-0.35963700	-0.20345800
C	4.77613300	-1.58668400	-0.07462000
C	4.94739800	0.75936600	-0.36320400
C	6.18931600	-1.66711200	-0.06911700
C	6.37551800	0.68849700	-0.33138300
N	4.46994700	2.02870200	-0.65005000
C	7.04778300	-0.53965300	-0.16578000
N	6.67261200	-2.95327100	0.10726600
C	8.47628400	-0.78479700	-0.16045900
H	8.77706600	-1.75490800	-0.54836400
C	9.51205900	-0.02338200	0.28951900
C	9.37356500	1.18087800	1.04175100
C	10.89123100	-0.56439100	0.07469700

N	9.26910900	2.14168200	1.69141400
O	11.13998400	-1.59461500	-0.51491400
O	11.83830000	0.23145100	0.61184400
H	12.69193100	-0.19388900	0.42546800
N	-1.60791100	0.02129100	-0.05114500
C	-4.27070500	5.08700200	0.48675200
C	-4.68316900	5.90195800	-0.59197500
C	-4.54992600	5.55794200	1.78009200
C	-5.33858400	7.12091000	-0.37214900
C	-5.19730000	6.76204400	2.02023100
H	-4.22335100	4.96079000	2.62591300
C	-5.59445900	7.55000800	0.93577500
H	-5.64942700	7.72414100	-1.21240500
H	-5.39257200	7.11231400	3.02732700
C	-4.90239000	-4.67519700	-0.41379900
C	-5.35566100	-5.43131600	0.69109600
C	-5.30611500	-5.10871500	-1.68721000
C	-6.16851100	-6.55915700	0.51494300
C	-6.11019100	-6.22284900	-1.88417000
H	-4.95346900	-4.55721600	-2.55333600
C	-6.54464700	-6.95411300	-0.77456200
H	-6.50737100	-7.11808200	1.37479400
H	-6.40107100	-6.54652700	-2.87698900
O	-6.22099400	8.72200300	1.24526500
O	-4.42533400	5.42723500	-1.84796000
O	-7.32778100	-8.03892300	-1.04213100
O	-4.97452800	-4.99158200	1.92833400

C	-6.63843600	9.57022300	0.18805400
H	-7.10143800	10.43660300	0.66237200
H	-5.79016100	9.90538100	-0.42261800
H	-7.37580300	9.07901800	-0.46001500
C	-4.86941400	6.16924500	-2.97186100
H	-5.95997100	6.29127200	-2.97165700
H	-4.39637900	7.15843800	-3.02028800
H	-4.57424200	5.58940900	-3.84747600
C	-5.45477200	-5.66613000	3.07964500
H	-6.55068200	-5.64786000	3.13211800
H	-5.10985400	-6.70747000	3.11589000
H	-5.04630000	-5.12508500	3.93430600
C	-7.79449900	-8.82536700	0.04196100
H	-8.38729000	-9.62679200	-0.40104200
H	-6.96530100	-9.26445600	0.61159000
H	-8.42935700	-8.24326600	0.72242400
S	6.98502000	2.27075400	-0.67219400
S	4.16138600	-3.19209700	0.17496000
N	5.79326100	-3.84973100	0.24038600
N	5.34554300	2.91175400	-0.84694600

Table S6: Cartesian coordinates of MS3 dye in the singlet open-shell ground-state, optimized with UB3LYP functional and 6-31G(d, p) basis set.

Atom symbol	X	Y	Z
C	5.67739700	-1.11683400	0.11201100
C	5.54308200	-2.24376600	-0.71247700
C	6.81133300	-1.00964700	0.92741000

C	6.50980700	-3.24300400	-0.70735100
H	4.67373600	-2.33414500	-1.35569200
C	7.78142200	-2.00684600	0.91358100
H	6.93424500	-0.13764000	1.56118100
C	7.65397200	-3.15059300	0.10558700
H	6.38323200	-4.10449900	-1.35162700
H	8.66278900	-1.89220700	1.53715000
C	5.12942500	1.27271200	0.01343700
C	4.61497700	2.25296000	0.87491500
C	6.10138800	1.64282200	-0.92486000
C	5.05007600	3.57051500	0.78685000
H	3.86790800	1.97729200	1.61215600
C	6.54273700	2.96041500	-0.99424700
H	6.51675700	0.89262000	-1.58958100
C	6.02514200	3.95855700	-0.14977800
H	4.63631400	4.31005000	1.46144900
H	7.31284200	3.22006300	-1.71416500
C	3.32802700	-0.39315500	0.18384600
C	2.88182200	-1.54722200	0.86343800
C	2.35642600	0.43916500	-0.41171900
C	1.53381400	-1.84967700	0.93807200
H	3.60446100	-2.19393400	1.34725000
C	1.01022900	0.12939800	-0.32815400
H	2.67106900	1.32262200	-0.95472400
C	0.55220500	-1.02381600	0.34583900
H	1.22998100	-2.72779100	1.49827000
H	0.29670600	0.78004300	-0.82501400

C	-0.85721900	-1.35754600	0.43500700
C	-1.43022500	-2.56973200	0.81182400
S	-2.10253000	-0.18768500	0.05327300
C	-2.82681000	-2.56822700	0.78780400
H	-0.84755700	-3.44517200	1.07182100
C	-3.39595500	-1.34898100	0.39197000
C	-4.78403200	-1.03093300	0.26761800
C	-5.84509400	-1.95545700	0.55571100
C	-5.26569900	0.24915200	-0.15878700
C	-7.26633100	-1.60491800	0.41549600
N	-5.66723000	-3.21670600	0.97569500
C	-6.68864900	0.59544100	-0.29777300
N	-4.45032800	1.26378400	-0.47511700
C	-7.74215300	-0.32955100	-0.01360500
N	-8.08118700	-2.62155600	0.73689000
S	-7.14447200	-3.88848000	1.17188700
N	-6.86401900	1.86102400	-0.71499700
S	-5.38531600	2.53182000	-0.90688200
C	-9.14064500	-0.01304800	-0.14440600
C	-9.70479500	1.20535500	-0.55796600
S	-10.41815700	-1.16382500	0.21201100
C	-11.09971400	1.21414000	-0.58725400
C	-11.67077600	0.00119200	-0.19694100
H	-11.68398400	2.07554000	-0.88326000
C	-13.02721500	-0.41192500	-0.08600900
H	-13.20367700	-1.43271100	0.24806900
C	-14.18480300	0.28386800	-0.33784500

C	-14.21139600	1.63537000	-0.78497300
C	-15.46786300	-0.42949100	-0.12631000
N	-14.20388700	2.74208200	-1.15054000
O	-15.56945200	-1.58115500	0.25239000
O	-16.54105700	0.34666300	-0.40308500
H	-17.32146800	-0.20665100	-0.23495700
H	-3.43671000	-3.42337900	1.03841000
H	-9.09161900	2.05216000	-0.82635500
N	4.69282400	-0.08338300	0.10451700
C	6.47809300	5.36517900	-0.29664700
C	6.76814000	6.20378400	0.80370700
C	6.65638200	5.91491900	-1.57678000
C	7.21140000	7.51997600	0.61694400
C	7.09388400	7.21572600	-1.78422400
H	6.41951300	5.29815600	-2.43827100
C	7.37337700	8.02492200	-0.67885200
H	7.43230300	8.14024000	1.47312300
H	7.21399500	7.62364100	-2.78134500
C	8.68188600	-4.22079300	0.16449700
C	9.18329800	-4.87609800	-0.98322800
C	9.21853600	-4.61099700	1.40238600
C	10.16886900	-5.86709400	-0.88147000
C	10.19441000	-5.59032700	1.52578400
H	8.83465900	-4.13755700	2.30082900
C	10.67343400	-6.22353200	0.37499000
H	10.54100300	-6.34982700	-1.77314500
H	10.58723300	-5.88382500	2.49254700

O	7.79461400	9.29262600	-0.95649000
O	6.61108800	5.65538200	2.04633900
O	11.62841200	-7.17823400	0.57073900
O	8.66984600	-4.47725300	-2.18604500
C	8.08699200	10.16449900	0.12330900
H	8.39569400	11.10865300	-0.32746900
H	7.20600700	10.33870800	0.75446700
H	8.90483900	9.77968300	0.74618100
C	6.95169200	6.42352700	3.18870700
H	8.00793100	6.72076000	3.17683700
H	6.32613900	7.32093300	3.27822400
H	6.77161200	5.77599500	4.04796300
C	9.18367700	-5.04566200	-3.37934200
H	10.25886900	-4.85547000	-3.48836700
H	9.00275100	-6.12719000	-3.42692800
H	8.64924700	-4.55830500	-4.19598400
C	12.15124900	-7.85936900	-0.55809700
H	12.88524500	-8.56655800	-0.16942800
H	11.37039600	-8.41163500	-1.09675100
H	12.64899900	-7.17098800	-1.25327400

Table S7: Cartesian coordinates of MS4 dye in the singlet open-shell ground-state, optimized with UB3LYP functional and 6-31G(d, p) basis set.

Atom symbol	X	Y	Z
C	-5.59338100	-1.17257000	-0.11005200
C	-5.38132800	-2.27250800	0.73387300
C	-6.73189700	-1.15683600	-0.92544200

C	-6.27708800	-3.33576100	0.74727000
H	-4.50711900	-2.29218600	1.37651900
C	-7.63109000	-2.21800800	-0.89330400
H	-6.91430300	-0.30625600	-1.57385000
C	-7.42492700	-3.33605500	-0.06580100
H	-6.09107700	-4.17557200	1.40548900
H	-8.51838700	-2.17509500	-1.51747200
C	-5.21926800	1.24966500	-0.03784200
C	-4.79976000	2.25180200	-0.92491500
C	-6.19696100	1.55865100	0.91611100
C	-5.33293100	3.53348900	-0.84635400
H	-4.04972200	2.02157800	-1.67466300
C	-6.73629400	2.83971900	0.97671100
H	-6.53973300	0.78904500	1.59979500
C	-6.31468100	3.86064200	0.10642300
H	-4.99201800	4.29156800	-1.54079700
H	-7.50882300	3.05141900	1.70958300
C	-3.30211000	-0.28200300	-0.20772200
C	-2.77867700	-1.42314700	-0.85683200
C	-2.39114300	0.64140600	0.35265500
C	-1.41403100	-1.62729200	-0.93935500
H	-3.45712500	-2.13960800	-1.30474000
C	-1.02682200	0.43131200	0.26288800
H	-2.76763500	1.51630400	0.86898800
C	-0.49992200	-0.70549400	-0.38366700
H	-1.02131500	-2.49912500	-1.45009500
H	-0.35861000	1.15595500	0.71953200

C	0.92286500	-0.95512000	-0.49531800
S	2.14089800	0.15928300	0.11981200
C	2.77219700	-2.03458500	-1.04402000
C	3.40406700	-0.93708800	-0.44356400
C	4.80610100	-0.69793800	-0.29024500
C	5.82456300	-1.59349400	-0.75467500
C	5.33723500	0.46725200	0.34613800
C	7.25905700	-1.32361800	-0.58435900
N	5.59029700	-2.75507100	-1.38409200
C	6.77370000	0.73512600	0.51534000
N	4.56268100	1.43676600	0.85438500
C	7.78798100	-0.16022500	0.05109800
N	8.02883600	-2.29752500	-1.09517800
S	7.03700600	-3.43338000	-1.72396600
N	7.00083200	1.90046100	1.14631900
S	5.55065400	2.57416900	1.48362100
C	9.19948500	0.08131900	0.20557500
C	9.81379700	1.18869000	0.81288200
S	10.42777700	-1.03166000	-0.37327800
C	11.20872700	1.14533500	0.81320800
C	11.72782600	0.00090300	0.20521600
H	11.82884200	1.92148600	1.24211700
C	13.06694800	-0.43253000	-0.00562700
H	13.20030700	-1.38456100	-0.51608600
C	14.25220600	0.16933100	0.33844900
C	14.33526200	1.42032200	1.01347300
C	15.50560000	-0.53900200	-0.02184400

N	14.37386900	2.44565300	1.56621400
O	15.55785500	-1.60929500	-0.59725900
O	16.60982600	0.14077300	0.36277200
H	17.36777300	-0.39936800	0.08469000
H	3.31946400	-2.85960100	-1.47688200
H	9.23662700	1.99570400	1.23804400
N	-4.68324700	-0.07169500	-0.12035500
C	-6.87138700	5.23056400	0.24299200
C	-7.24932500	6.02611700	-0.86265400
C	-7.06364200	5.78574600	1.51874200
C	-7.78911400	7.30705500	-0.68504300
C	-7.59571400	7.05223700	1.71706300
H	-6.76123500	5.20314300	2.38349900
C	-7.96129500	7.81916600	0.60663000
H	-8.07610000	7.89426200	-1.54493600
H	-7.72531400	7.46600400	2.71057400
C	-8.37661700	-4.47535400	-0.10522000
C	-8.82976000	-5.14559500	1.05389200
C	-8.88629200	-4.92150400	-1.33562000
C	-9.74394600	-6.20434400	0.97003400
C	-9.79167600	-5.96821600	-1.44125900
H	-8.53696800	-4.43727300	-2.24234800
C	-10.22392600	-6.61496000	-0.27949500
H	-10.08034300	-6.69764900	1.87005900
H	-10.16395600	-6.30394100	-2.40238200
O	-8.47333300	9.05486300	0.87537200
O	-7.07719500	5.47112500	-2.10024900

O	-11.11027900	-7.63676000	-0.45800100
O	-8.34420400	-4.69270800	2.24909900
C	-8.85805600	9.88309600	-0.20987800
H	-9.22938600	10.80764600	0.23422500
H	-8.00827100	10.11501500	-0.86478800
H	-9.65733800	9.42518000	-0.80682600
C	-7.50245800	6.19104600	-3.24573700
H	-8.57820400	6.40506000	-3.21329400
H	-6.95131200	7.13286800	-3.36344600
H	-7.29142800	5.54514200	-4.09913600
C	-8.81330200	-5.27876400	3.45227000
H	-9.89895700	-5.16345100	3.56261100
H	-8.55617300	-6.34397200	3.51449200
H	-8.31243800	-4.74311400	4.25988700
C	-11.58105700	-8.33640300	0.68239100
H	-12.26402700	-9.09940700	0.30649000
H	-10.76182300	-8.82397200	1.22642200
H	-12.12473800	-7.67474500	1.36907400
N	1.42697700	-2.03952000	-1.06960100

Table S8: Cartesian coordinates of MS5 dye in the singlet open-shell ground-state, optimized with UB3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*
C	-5.59497100	-1.15036600	-0.10424000
C	-5.39636100	-2.24981800	0.74348500
C	-6.73377900	-1.12239300	-0.91875900
C	-6.30589300	-3.30124800	0.76137000

H	-4.52204700	-2.27841800	1.38567100
C	-7.64654200	-2.17175400	-0.88234100
H	-6.90565200	-0.27161500	-1.56978100
C	-7.45421700	-3.28946600	-0.05098600
H	-6.13045000	-4.14100900	1.42252000
H	-8.53375100	-2.11950900	-1.50588800
C	-5.19106700	1.26700400	-0.03534700
C	-4.76632000	2.26214300	-0.92768600
C	-6.15863600	1.58882200	0.92454900
C	-5.28434900	3.54997600	-0.84832600
H	-4.02427400	2.02168600	-1.68217600
C	-6.68282400	2.87609700	0.98609600
H	-6.50542900	0.82453100	1.61216100
C	-6.25559300	3.89031500	0.11063600
H	-4.93975400	4.30262400	-1.54680700
H	-7.44786800	3.09812800	1.72371200
C	-3.29353000	-0.28798300	-0.21083900
C	-2.78628100	-1.43995700	-0.85434600
C	-2.36891500	0.62880900	0.33895100
C	-1.42473100	-1.66030700	-0.94200500
H	-3.47502200	-2.15149100	-1.29422200
C	-1.00789000	0.40209800	0.24449900
H	-2.73269400	1.51143900	0.85112300
C	-0.49718200	-0.74527100	-0.39691500
H	-1.04462100	-2.54001500	-1.44874100
H	-0.32919400	1.12186200	0.69332100
C	0.92139600	-1.01185200	-0.51369100

S	2.15531100	0.09256200	0.08714100
C	2.75485600	-2.11701200	-1.06418400
C	3.40255300	-1.02252900	-0.47472300
C	4.80774600	-0.79868600	-0.33031900
C	5.81372400	-1.70952500	-0.79338600
C	5.35521100	0.36513600	0.29488900
C	7.25205100	-1.45479800	-0.63222800
N	5.56388900	-2.87324400	-1.41317200
C	6.79470600	0.61638200	0.45411400
N	4.59663700	1.34887200	0.80084700
C	7.79339500	-0.29334700	-0.00836600
N	8.00985800	-2.44107600	-1.13960100
S	7.00099500	-3.56952300	-1.75472200
N	7.04270100	1.78299200	1.07508700
S	5.60332700	2.47715000	1.41552300
C	9.20729900	-0.06663100	0.13734800
C	9.85186600	1.03314000	0.73082100
S	10.44217500	-1.17264900	-0.42531000
C	11.67781600	-0.07033800	0.18012200
C	13.06003400	-0.40233300	0.02964200
H	13.29375800	-1.34264200	-0.46324800
C	14.15148100	0.31600600	0.42920300
C	14.10441500	1.57706200	1.09485500
C	15.48599800	-0.28293900	0.13688200
N	14.13129500	2.60572700	1.63892600
O	15.65483700	-1.34862300	-0.42351300
O	16.50513200	0.49101600	0.56473600

H	17.32038900	0.01786300	0.32944000
H	3.29038400	-2.95140900	-1.49388000
H	9.31496900	1.86546200	1.16144100
N	-4.67083300	-0.06091700	-0.11871600
C	-6.79561400	5.26673900	0.24811200
C	-7.17080700	6.06484100	-0.85666000
C	-6.97375500	5.82617000	1.52410400
C	-7.69452400	7.35225900	-0.67796800
C	-7.48971000	7.09908800	1.72342400
H	-6.67292300	5.24158600	2.38806900
C	-7.85294500	7.86846500	0.61384700
H	-7.97977200	7.94140900	-1.53710400
H	-7.60841600	7.51601500	2.71696500
C	-8.42071800	-4.41631000	-0.08559600
C	-8.88127600	-5.07671300	1.07626200
C	-8.93754900	-4.85974300	-1.31402400
C	-9.80942500	-6.12356900	0.99685300
C	-9.85661700	-5.89483700	-1.41522500
H	-8.58293000	-4.38315400	-2.22274300
C	-10.29611600	-6.53197200	-0.25081500
H	-10.15132600	-6.60941900	1.89885400
H	-10.23432700	-6.22884700	-2.37481800
O	-8.34881700	9.11035900	0.88355900
O	-7.01265400	5.50587200	-2.09429500
O	-11.19598200	-7.54247100	-0.42501800
O	-8.38846600	-4.62632700	2.26938700
C	-8.72986400	9.94169300	-0.20071100

H	-9.08755800	10.87118600	0.24422900
H	-7.88110400	10.16251600	-0.86073400
H	-9.53797500	9.49250600	-0.79235800
C	-7.43633500	6.22891400	-3.23849600
H	-8.50925600	6.45562100	-3.19988600
H	-6.87481300	7.16393500	-3.36109900
H	-7.23809800	5.57914800	-4.09202300
C	-8.86414000	-5.20195900	3.47509800
H	-9.94804300	-5.07183000	3.58599200
H	-8.62107700	-6.27024400	3.54073100
H	-8.35541600	-4.67019500	4.28035500
C	-11.67518900	-8.23190400	0.71815900
H	-12.36864800	-8.98689900	0.34534100
H	-10.86211100	-8.72859900	1.26314300
H	-12.20935100	-7.56064000	1.40296100
N	1.41012400	-2.10658800	-1.08301200
N	11.19458200	1.02217300	0.74930800

Table S9: Cartesian coordinates of MS6 dye in the singlet open-shell ground-state, optimized with UB3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*
C	-7.41045400	1.18728100	0.05274000
C	-7.07700000	2.26739000	-0.77801000
C	-8.50024900	1.31881000	0.92305400
C	-7.80418600	3.45130100	-0.72555400
H	-6.24065600	2.17531400	-1.46337700
C	-9.23253800	2.50139200	0.95631400

H	-8.77736600	0.48750700	1.56284700
C	-8.90074900	3.59916600	0.14278400
H	-7.52600000	4.27193800	-1.37557600
H	-10.08676000	2.57272400	1.62269700
C	-7.39113900	-1.26402500	-0.06545000
C	-7.05178000	-2.33922800	0.76921500
C	-8.46775300	-1.41157400	-0.94941300
C	-7.76033200	-3.53391200	0.70744800
H	-6.22521000	-2.23511500	1.46463300
C	-9.18178300	-2.60499600	-0.99194000
H	-8.74926100	-0.58439100	-1.59262700
C	-8.84370100	-3.69790300	-0.17449300
H	-7.47766300	-4.35059800	1.36047000
H	-10.02643000	-2.68892500	-1.66896800
C	-5.26899500	-0.02178500	0.00604600
C	-4.55351100	0.99830300	0.66838500
C	-4.52923400	-1.03068400	-0.64439700
C	-3.16932700	1.00626500	0.67354200
H	-5.09626000	1.77430100	1.19551600
C	-3.14424600	-1.01518300	-0.63092000
H	-5.05171500	-1.81858800	-1.17416300
C	-2.41944100	0.00270000	0.02280100
H	-2.65631300	1.78683300	1.22601400
H	-2.61181700	-1.79282500	-1.17093900
C	5.10020400	0.17941000	0.06379900
C	5.89257200	1.33558500	0.36263800
C	5.89748900	-0.97668900	-0.24022800

C	7.36320300	1.35567600	0.36229200
N	5.35721900	2.52216600	0.67455300
C	7.36786200	-0.95262400	-0.23960700
N	5.40575000	-2.18418900	-0.55286800
C	8.15464100	0.20185800	0.05823500
N	7.85397700	2.56611700	0.67621100
S	6.58628600	3.56621900	0.94226000
N	7.90177900	-2.14250500	-0.55171500
S	6.67171500	-3.18562900	-0.81867800
C	15.63958100	0.45776100	0.09360700
H	16.05323900	1.43209700	0.34654800
C	16.60124300	-0.48983500	-0.15833300
C	16.30570900	-1.83724400	-0.50923400
C	18.01880800	-0.06459300	-0.05343800
N	16.02779700	-2.93273300	-0.79433700
O	18.38739500	1.05721000	0.23827800
O	18.87928300	-1.07300100	-0.32100000
H	19.77041200	-0.69800800	-0.22690900
N	-6.67216000	-0.03277400	-0.00148200
C	-9.59150500	-4.97546200	-0.29407700
C	-9.99692200	-5.74228500	0.82199000
C	-9.94685500	-5.46457800	-1.56176100
C	-10.71827500	-6.93302300	0.66197000
C	-10.66053000	-6.64129500	-1.74287300
H	-9.62855600	-4.90488100	-2.43590100
C	-11.04909800	-7.38164000	-0.62239200
H	-11.02206300	-7.49921200	1.53013900

H	-10.91493100	-7.00628400	-2.73138700
C	-9.66914600	4.86535200	0.25253100
C	-10.07274100	5.62535800	-0.86885100
C	-10.04721900	5.34958100	1.51550200
C	-10.81405700	6.80503100	-0.71832900
C	-10.78088400	6.51537400	1.68722500
H	-9.73121800	4.79505300	2.39376800
C	-11.16716000	7.24916700	0.56165300
H	-11.11599200	7.36606400	-1.59048600
H	-11.05291400	6.87680500	2.67234800
O	-11.74334700	-8.52909900	-0.87442900
O	-9.66415400	-5.24972400	2.05340700
O	-11.88177800	8.38604900	0.80455400
O	-9.71757200	5.13740200	-2.09583300
C	-12.15927200	-9.32728000	0.22159800
H	-12.68369700	-10.18102000	-0.20976000
H	-11.30468500	-9.68923800	0.80773700
H	-12.84431300	-8.78254300	0.88412000
C	-10.10302000	-5.93647500	3.21381000
H	-11.19758500	-6.00208500	3.25617000
H	-9.67928300	-6.94716400	3.27460700
H	-9.74656000	-5.34873000	4.06090000
C	-10.15489000	5.81544700	-3.26194200
H	-11.24984000	5.86339500	-3.31611600
H	-9.74682500	6.83275100	-3.31974400
H	-9.77994300	5.23236700	-4.10425900
C	-12.29754400	9.17668600	-0.29699200

H	-12.84024900	10.02243300	0.12744300
H	-11.44206000	9.55156100	-0.87363600
H	-12.96625900	8.62069400	-0.96679200
C	3.67081500	0.18216800	0.06890400
C	2.82407300	-0.90126400	-0.21529400
C	1.47263100	-0.56402900	-0.11957300
C	1.22884400	0.77029500	0.23632300
C	-0.96586000	0.03058800	0.03376400
C	-0.13605200	1.10560100	0.32043400
H	3.21274200	-1.87404400	-0.47587000
H	-0.51169000	2.09474700	0.54908700
S	-0.02991200	-1.43001400	-0.34021900
S	2.71665900	1.64710600	0.45910100
C	14.22143400	0.35054400	0.07172300
C	13.38716400	-0.73423600	-0.20841700
C	12.03214800	-0.39305500	-0.11342300
C	11.79012200	0.94640000	0.23790800
C	9.59382500	0.20103500	0.05221700
C	10.43288700	1.28435200	0.33201500
H	13.76445500	-1.71486600	-0.46651500
H	10.04539100	2.25821400	0.58833500
S	10.53765000	-1.26639900	-0.33535000
S	13.27959500	1.81212500	0.45801800

Table S10: Cartesian coordinates of MS7 dye in the singlet open-shell ground-state, optimized with UB3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*

C	-7.25560300	-1.23458200	-0.00412800
C	-6.90035100	-2.26643700	0.87675700
C	-8.28936100	-1.45706800	-0.92225600
C	-7.55159400	-3.49391000	0.82671700
H	-6.10656000	-2.10320300	1.59852400
C	-8.94661300	-2.68300900	-0.95371800
H	-8.58268700	-0.66289500	-1.60085500
C	-8.59140800	-3.73385600	-0.08961300
H	-7.25793000	-4.27679600	1.51521500
H	-9.75992500	-2.82628500	-1.65852200
C	-7.40332600	1.21250100	0.06064900
C	-7.12405600	2.28129100	-0.80350700
C	-8.50583400	1.30899200	0.91873000
C	-7.91756100	3.42303700	-0.79500300
H	-6.27795800	2.21416200	-1.47978900
C	-9.30401700	2.44865000	0.90852000
H	-8.74086700	0.48379800	1.58284900
C	-9.02779900	3.53626000	0.06120300
H	-7.68101300	4.23657400	-1.46985700
H	-10.16673600	2.49299400	1.56616900
C	-5.20130800	0.11622600	0.09115000
C	-4.39385000	-0.88863600	-0.48796700
C	-4.55804000	1.20817300	0.71450500
C	-3.01470300	-0.80290900	-0.44412200
H	-4.86350000	-1.73084000	-0.98221500
C	-3.17699800	1.28855900	0.75073000
H	-5.15373000	1.98475000	1.17904400

C	-2.36836200	0.28901400	0.17470000
H	-2.40593200	-1.57377400	-0.90286300
H	-2.72046500	2.13704500	1.25275800
C	5.04157700	0.11078700	0.04149100
C	5.77502300	-0.97726600	-0.53419000
C	5.89688400	1.13427900	0.57465800
C	7.24282600	-1.05498800	-0.58335800
N	5.18079400	-2.04089300	-1.08965100
C	7.36446800	1.05316300	0.52381400
N	5.46773400	2.25823000	1.16787200
C	8.09219000	-0.03292100	-0.05113300
N	7.67149900	-2.18123900	-1.17754200
S	6.35489600	-3.04350600	-1.62313300
N	7.95819100	2.11910400	1.08077500
S	6.78286600	3.12114500	1.61411000
C	15.55555700	-0.56755800	-0.37458500
H	15.91928100	-1.47461800	-0.85350600
C	16.56373000	0.25993600	0.05457100
C	16.33665900	1.50322100	0.70942200
C	17.95853800	-0.18536400	-0.18760900
N	16.11437300	2.51546600	1.24279300
O	18.26953300	-1.22538800	-0.73599400
O	18.86860400	0.70207300	0.27342800
H	19.74008100	0.32432400	0.06981500
N	-6.59819700	0.03260300	0.04931100
C	-9.86769500	4.75945000	0.12390200
C	-10.30287100	5.45905100	-1.02467500

C	-10.28434300	5.26141300	1.36770000
C	-11.11098200	6.59894300	-0.91806400
C	-11.08396900	6.38868700	1.49592100
H	-9.94572900	4.75419900	2.26590500
C	-11.50040900	7.06309000	0.34416700
H	-11.43599100	7.11376000	-1.81019500
H	-11.38500400	6.76559300	2.46668800
C	-9.27614900	-5.04736800	-0.19614700
C	-9.68869200	-5.79847900	0.92796700
C	-9.56082900	-5.58958600	-1.46008900
C	-10.34955200	-7.02520400	0.77908400
C	-10.21357900	-6.80267600	-1.63010400
H	-9.23474500	-5.04223000	-2.33914800
C	-10.61097800	-7.52641900	-0.50183100
H	-10.66044300	-7.57876600	1.65286200
H	-10.41348100	-7.20828300	-2.61528900
O	-12.27998400	8.16475400	0.54473400
O	-9.90930900	4.95296800	-2.23231800
O	-11.24319900	-8.71127600	-0.74298800
O	-9.42521800	-5.25479600	2.15455500
C	-12.72862200	8.89584100	-0.58481400
H	-13.32147300	9.72288300	-0.19180600
H	-11.88981300	9.29950500	-1.16644600
H	-13.35904200	8.28248900	-1.24153400
C	-10.37219000	5.56814000	-3.42331000
H	-11.46747400	5.55224700	-3.48810300
H	-10.02136600	6.60451100	-3.51014200

H	-9.95642200	4.98090200	-4.24325900
C	-9.87447500	-5.92735000	3.31939000
H	-10.96574000	-6.04243600	3.32529500
H	-9.40771900	-6.91501600	3.42580100
H	-9.57615300	-5.29937400	4.16004300
C	-11.66441800	-9.49501600	0.36148900
H	-12.13352300	-10.38413900	-0.06199400
H	-10.81737800	-9.80011500	0.98941300
H	-12.39769400	-8.96282500	0.98117700
C	3.61203600	0.16636300	0.07828600
C	2.82598400	1.19629700	0.62264000
C	1.45848100	0.94477600	0.49727600
C	1.15524800	-0.26729000	-0.13717600
C	-0.92078800	0.34497900	0.19601800
H	3.26840400	2.06882800	1.07805000
S	-0.03831100	1.73578600	0.91634100
S	2.58978900	-1.13794300	-0.60073300
C	14.14409800	-0.41253700	-0.28497000
C	13.36625200	0.61238200	0.25832400
C	11.99529800	0.35493600	0.13071800
C	11.68576400	-0.85939700	-0.50602200
C	9.52996700	-0.08988400	-0.08927700
C	10.31285300	-1.11364800	-0.63196200
H	13.79283800	1.49341500	0.71916100
H	9.87647900	-1.98814000	-1.08927500
S	10.54710400	1.21311600	0.59008900
S	13.12956000	-1.71039400	-0.96161300

N	-0.14027400	-0.59622300	-0.30234000

Table S11: Cartesian coordinates of MS8 dye in the singlet open-shell ground-state, optimized with UB3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*
C	-7.24428800	-1.20940500	0.00352700
C	-6.89721600	-2.24340500	0.88510800
C	-8.28286300	-1.42243000	-0.91134000
C	-7.56127900	-3.46413700	0.83882700
H	-6.09983600	-2.08720400	1.60447900
C	-8.95278700	-2.64157900	-0.93910400
H	-8.56988800	-0.62623100	-1.59026200
C	-8.60603500	-3.69470700	-0.07430800
H	-7.27389500	-4.24893400	1.52778300
H	-9.76954700	-2.77750900	-1.64135600
C	-7.36759700	1.23897000	0.06773800
C	-7.08350200	2.30349500	-0.80004500
C	-8.46377400	1.34718200	0.93242600
C	-7.86603300	3.45276600	-0.78855800
H	-6.24235300	2.22712500	-1.48150900
C	-9.25105800	2.49441400	0.92529700
H	-8.70252800	0.52528000	1.59929800
C	-8.96972200	3.57797800	0.07444600
H	-7.62601400	4.26289100	-1.46626600
H	-10.10922900	2.54805200	1.58816300
C	-5.17646800	0.12109100	0.08893900
C	-4.38132800	-0.89412700	-0.48960800

C	-4.51962000	1.20917900	0.70531700
C	-3.00137100	-0.82183700	-0.45200700
H	-4.86135000	-1.73349300	-0.97864300
C	-3.13787600	1.27589900	0.73550200
H	-5.10555600	1.99334700	1.16945100
C	-2.34153400	0.26610100	0.15986600
H	-2.40223600	-1.60040800	-0.91040800
H	-2.67085100	2.12162800	1.23249900
C	5.06442100	0.01379600	-0.00415500
C	5.78511000	-1.08440800	-0.57706800
C	5.93215600	1.03175600	0.51965500
C	7.25189700	-1.17677800	-0.63225400
N	5.17786800	-2.14498100	-1.12400400
C	7.39833200	0.93601800	0.46272800
N	5.51665600	2.16305900	1.10858800
C	8.11373700	-0.16009100	-0.10940100
N	7.66626300	-2.31070700	-1.22229700
S	6.33915700	-3.16210700	-1.65722400
N	8.00435500	1.99927200	1.01126500
S	6.84180200	3.01548100	1.54422100
C	15.49496000	-0.46888800	-0.30858500
H	15.97108900	-1.33556800	-0.75978800
C	16.36313200	0.47113000	0.17305900
C	15.97869300	1.68981500	0.80577200
C	17.81651600	0.17775700	0.01313200
N	15.71800400	2.69687000	1.32825700
O	18.26228000	-0.82581800	-0.50862300

O	18.59883500	1.15566400	0.51472100
H	19.51597500	0.87302800	0.36336600
N	-6.57382300	0.05123300	0.05332800
C	-9.79740000	4.80926100	0.14041300
C	-10.23258500	5.51154200	-1.00653400
C	-10.20170000	5.31687000	1.38601500
C	-11.02892100	6.65937000	-0.89665000
C	-10.98948200	6.45204700	1.51744900
H	-9.86264500	4.80762200	2.28290100
C	-11.40622700	7.12896900	0.36725200
H	-11.35424300	7.17616100	-1.78752200
H	-11.28097400	6.83319000	2.48947000
C	-9.30463600	-5.00118900	-0.17683300
C	-9.72146700	-5.74637200	0.94965700
C	-9.59875600	-5.54222300	-1.43913600
C	-10.39539900	-6.96640800	0.80455500
C	-10.26445800	-6.74875200	-1.60538500
H	-9.26973400	-4.99953900	-2.31999600
C	-10.66586600	-7.46674500	-0.47483100
H	-10.70933700	-7.51547500	1.68007500
H	-10.47153400	-7.15369800	-2.58935600
O	-12.17376100	8.23838900	0.57096100
O	-9.85120300	5.00006500	-2.21579100
O	-11.31095400	-8.64531500	-0.71232900
O	-9.44868300	-5.20368000	2.17461900
C	-12.62181600	8.97259200	-0.55684300
H	-13.20408300	9.80592500	-0.16133100

H	-11.78248300	9.36721300	-1.14388100
H	-13.26217400	8.36474300	-1.20903700
C	-10.31506700	5.61827100	-3.40487500
H	-11.41081100	5.61304400	-3.46315900
H	-9.95458700	6.65102000	-3.49511200
H	-9.90993900	5.02593600	-4.22647800
C	-9.90156600	-5.86974900	3.34182500
H	-10.99393300	-5.97350700	3.35097100
H	-9.44473300	-6.86201100	3.44846100
H	-9.59436900	-5.24357600	4.18061800
C	-11.73683200	-9.42318900	0.39455000
H	-12.21633900	-10.30800800	-0.02627300
H	-10.89103100	-9.73610300	1.02028200
H	-12.46269500	-8.88262000	1.01569700
C	3.63614000	0.08328600	0.03842100
C	2.86251600	1.12382600	0.58127500
C	1.49244300	0.88542400	0.46306000
C	1.17439000	-0.32690200	-0.16444200
C	-0.89382200	0.30786400	0.17482700
H	3.31571900	1.99405600	1.03049300
S	0.00541800	1.69327400	0.88465900
S	2.59802100	-1.21411900	-0.62984000
C	14.06871500	-0.44818700	-0.29001200
C	12.00935600	0.18912100	0.05123600
C	11.69237000	-1.02959700	-0.57865300
C	9.55081800	-0.23032800	-0.15322300
C	10.31762000	-1.26937400	-0.69572100

H	9.86560200	-2.13989200	-1.14453400
S	10.57777200	1.07151500	0.51616000
S	13.16896600	-1.83065700	-1.00156000
N	-0.12469500	-0.64365900	-0.32248900
N	13.30000900	0.50534300	0.20820800

Table S12: Cartesian coordinates of MS9 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*
C	-5.69044000	-1.06556000	-0.09267800
C	-5.61422700	-2.18644300	0.74757600
C	-6.78731100	-0.94600300	-0.95597700
C	-6.59968400	-3.16668700	0.71171500
H	-4.77424700	-2.28756200	1.42719100
C	-7.77758800	-1.92333000	-0.97237900
H	-6.86620900	-0.07896900	-1.60345400
C	-7.70711800	-3.06053600	-0.14872300
H	-6.51706600	-4.02378400	1.36903400
H	-8.62966000	-1.79802800	-1.63361900
C	-5.09210000	1.31342700	-0.00664900
C	-4.50455200	2.26967100	-0.84836100
C	-6.10545000	1.72154900	0.87034500
C	-4.90916700	3.59903900	-0.80054600
H	-3.72348000	1.96606800	-1.53783300
C	-6.51623400	3.05065800	0.89833500
H	-6.57724200	0.99139300	1.51956900
C	-5.92577900	4.02408500	0.07348400

H	-4.43784100	4.31899700	-1.45850600
H	-7.31889600	3.33922600	1.57020000
C	-3.32321800	-0.39641300	-0.06629300
C	-2.87199300	-1.55653500	-0.72871800
C	-2.36561600	0.40864600	0.58289500
C	-1.52782800	-1.89230000	-0.73539100
H	-3.58457000	-2.18263400	-1.25314500
C	-1.02255000	0.06672200	0.56656600
H	-2.68668800	1.29709900	1.11407000
C	-0.56328100	-1.09296800	-0.08875600
H	-1.21211300	-2.77266400	-1.28635800
H	-0.31882400	0.69476200	1.10534700
C	0.84619400	-1.46611300	-0.10902400
C	1.39766500	-2.71929300	-0.32069600
S	2.10431500	-0.28528400	0.16918600
C	2.80335300	-2.72915600	-0.27412100
H	0.80249200	-3.61277800	-0.46432700
C	3.37731900	-1.48818400	-0.02325800
C	4.79108600	-1.17587600	0.05120700
C	5.80096000	-2.00037000	-0.49908000
C	5.30849500	-0.00299600	0.66333900
C	7.18259800	-1.68595600	-0.40327600
C	6.69590700	0.30637500	0.76949200
N	4.48872600	0.97089100	1.19986700
C	7.69948800	-0.53736800	0.25218200
N	7.99805300	-2.59898000	-1.04492200
C	9.12559500	-0.25471100	0.35859700

C	9.73872500	0.61686400	1.25824000
S	10.32810400	-0.97065300	-0.68737600
C	11.12812100	0.72819900	1.10345900
C	11.62420300	-0.06177700	0.07177300
H	11.75055600	1.35381900	1.72914400
C	12.95266200	-0.25639200	-0.41997600
H	13.07648500	-0.97141200	-1.23122400
C	14.12377700	0.33209400	-0.02729300
C	14.20926500	1.30004600	1.01493000
C	15.36536100	-0.07431300	-0.73975900
N	14.24715700	2.08784700	1.87235900
O	15.40900900	-0.88674500	-1.64195100
O	16.45705800	0.56655300	-0.26935100
H	17.20980800	0.23994600	-0.78962100
H	3.37705800	-3.64283600	-0.36384000
H	9.20244300	1.13416100	2.04269700
N	-4.68572600	-0.05343900	-0.05568900
C	-6.34943200	5.44385100	0.17780300
C	-6.55951100	6.27337300	-0.94715300
C	-6.58085300	6.01644500	1.43910000
C	-6.97810700	7.60285500	-0.80174600
C	-6.99564800	7.33069900	1.60588400
H	-6.40571300	5.40630100	2.31985900
C	-7.19543800	8.13037700	0.47681100
H	-7.13735600	8.21588900	-1.67662400
H	-7.15785800	7.75580800	2.58980000
C	-8.75292700	-4.11132400	-0.24008200

C	-9.31792200	-4.74111300	0.89216000
C	-9.24219000	-4.50762200	-1.49538600
C	-10.31782200	-5.71399800	0.75928400
C	-10.23166300	-5.46905700	-1.64979100
H	-8.80959200	-4.05353400	-2.38161100
C	-10.77360100	-6.07723600	-0.51373200
H	-10.73858800	-6.17733100	1.63957600
H	-10.58746800	-5.76742000	-2.62934300
O	-7.59832000	9.41260100	0.71481800
O	-6.35093600	5.70310500	-2.17247500
O	-11.73840300	-7.01599700	-0.73961200
O	-8.84997000	-4.33635200	2.11166600
C	-7.80921800	10.27533600	-0.39064300
H	-8.11642300	11.23388800	0.02988500
H	-6.89150200	10.41737300	-0.97594100
H	-8.60248800	9.90267300	-1.05163400
C	-6.60949100	6.46319700	-3.34105200
H	-7.65676900	6.78735500	-3.39040200
H	-5.95700100	7.34328700	-3.40824800
H	-6.40039400	5.79928100	-4.18106300
C	-9.42805000	-4.87767600	3.28768800
H	-10.50302000	-4.66488800	3.34592200
H	-9.27168600	-5.96189000	3.35769200
H	-8.92090700	-4.38968900	4.12122400
C	-12.32376300	-7.67090300	0.37363800
H	-13.05409800	-8.36910800	-0.03764700
H	-11.57865700	-8.23072800	0.95365000

H	-12.83767500	-6.96348500	1.03731100
S	6.82041800	1.85106100	1.55237900
S	5.66970500	-3.45743200	-1.43387700
N	7.41189200	-3.55530200	-1.62350300
N	5.06290200	1.97916100	1.68856600

Table S13: Cartesian coordinates of MS10 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(d, p) basis set.

Atom symbol	X	Y	Z
C	-5.61064300	-1.12494000	-0.10612600
C	-5.44205600	-2.22511300	0.74727800
C	-6.73316100	-1.08661800	-0.94269000
C	-6.36388900	-3.26607700	0.74955100
H	-4.58047600	-2.26293600	1.40601200
C	-7.65936900	-2.12479700	-0.92121200
H	-6.88252300	-0.23557200	-1.59893500
C	-7.49637500	-3.24260400	-0.08417300
H	-6.21078900	-4.10655700	1.41549400
H	-8.53375900	-2.06356900	-1.56195300
C	-5.17645800	1.28790600	-0.04027000
C	-4.71360300	2.27455500	-0.92313200
C	-6.16416400	1.62792800	0.89255600
C	-5.21407100	3.57035000	-0.86092700
H	-3.95461000	2.02130800	-1.65629300
C	-6.67143800	2.92289600	0.93607500
H	-6.54049300	0.87121500	1.57301400
C	-6.20594400	3.92789000	0.06999100

H	-4.83904900	4.31586900	-1.55148600
H	-7.45261800	3.15845200	1.65239100
C	-3.29507900	-0.29323300	-0.16504400
C	-2.78852100	-1.44576300	-0.80487400
C	-2.37286800	0.60447200	0.41528600
C	-1.42698000	-1.68581100	-0.85916500
H	-3.47579800	-2.14469500	-1.26690000
C	-1.01162800	0.35950400	0.35161300
H	-2.73642100	1.48836400	0.92558900
C	-0.50315800	-0.78862900	-0.28511900
H	-1.04822600	-2.56831100	-1.36230300
H	-0.33520000	1.06668300	0.82384900
C	0.91998100	-1.07353000	-0.37181300
S	2.14829700	0.01984000	0.26001600
C	2.76298400	-2.18308200	-0.86802300
C	3.39740800	-1.09331600	-0.28754500
C	4.82235200	-0.86957900	-0.14572200
C	5.80383300	-1.56792700	-0.88732300
C	5.37604300	0.09005800	0.74180200
C	7.19564700	-1.34072000	-0.71428000
C	6.77250300	0.30919900	0.92296800
N	4.58714400	0.93003100	1.50424800
C	7.74821300	-0.41536400	0.20946800
N	7.98309200	-2.09578700	-1.56278500
C	9.18304800	-0.22402900	0.38478100
C	9.81846000	0.36268700	1.47842600
S	10.36798700	-0.69100300	-0.81075900

C	11.21257600	0.45787700	1.35701000
C	11.68868900	-0.05738100	0.15615500
H	11.85160700	0.87724800	2.12253700
C	13.01403400	-0.16795000	-0.37049600
H	13.11926900	-0.65424900	-1.33854800
C	14.20138200	0.25612300	0.15982300
C	14.31196000	0.91973500	1.41602600
C	15.43446200	0.00114700	-0.63414800
N	14.37001800	1.45866500	2.44720700
O	15.45644900	-0.55277200	-1.71497600
O	16.54360300	0.45868300	-0.01492100
H	17.28948500	0.24979600	-0.60150000
H	3.27728000	-3.05735400	-1.24797500
H	9.29392300	0.68011000	2.36994000
N	-4.67358300	-0.04717700	-0.10565900
C	-6.72886400	5.31293500	0.18905100
C	-7.06686900	6.11102100	-0.92748800
C	-6.92820700	5.88113300	1.45782500
C	-7.57562000	7.40688200	-0.76696600
C	-7.43038900	7.16242900	1.63945300
H	-6.65603000	5.29619400	2.33101100
C	-7.75642400	7.93153200	0.51845800
H	-7.83220100	7.99591900	-1.63519400
H	-7.56609700	7.58569600	2.62815100
C	-8.47544300	-4.35835300	-0.13471600
C	-8.97011400	-5.00636700	1.01992000
C	-8.97003700	-4.80260200	-1.37177300

C	-9.90908800	-6.04237200	0.92558700
C	-9.89970800	-5.82690800	-1.48794900
H	-8.58946800	-4.33515300	-2.27474300
C	-10.37288900	-6.45185200	-0.33038900
H	-10.27694800	-6.51883700	1.82239400
H	-10.26019500	-6.16150200	-2.45397200
O	-8.24043400	9.18229900	0.77090000
O	-6.88815000	5.54373400	-2.15876400
O	-11.28148000	-7.45258600	-0.51908300
O	-8.49830800	-4.55521000	2.22142000
C	-8.58334400	10.01323500	-0.32595900
H	-8.93762400	10.95036200	0.10563200
H	-7.71617700	10.21811500	-0.96702600
H	-9.38386000	9.57306200	-0.93457700
C	-7.27390300	6.26753200	-3.31543800
H	-8.34397100	6.51046300	-3.30334800
H	-6.69589000	7.19369900	-3.42893900
H	-7.06539400	5.61104000	-4.16138300
C	-9.00793700	-5.11785300	3.41902100
H	-10.09243800	-4.97399300	3.50493500
H	-8.77975700	-6.18871600	3.49620700
H	-8.51094200	-4.58772900	4.23268100
C	-11.79472300	-8.12841300	0.61710500
H	-12.48939800	-8.87702100	0.23367500
H	-11.00055300	-8.63194400	1.18339800
H	-12.33536100	-7.44619100	1.28589200
S	6.94601200	1.60211900	2.06892600

S	5.62796100	-2.74131100	-2.15387800
N	7.36839900	-2.85500300	-2.36114500
N	5.19448400	1.76014900	2.23075600
N	1.41180200	-2.17428300	-0.91376900

Table S14: Cartesian coordinates of MS11 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*
C	-5.60404200	-1.12178600	-0.09519800
C	-5.43194400	-2.21888500	0.76136600
C	-6.73259600	-1.08346300	-0.92347400
C	-6.35655600	-3.25731000	0.77464900
H	-4.56564500	-2.25631700	1.41392000
C	-7.66136500	-2.11906400	-0.89106600
H	-6.88456300	-0.23444400	-1.58175300
C	-7.49510100	-3.23401400	-0.05082100
H	-6.20087700	-4.09552000	1.44282900
H	-8.54040200	-2.05795000	-1.52540600
C	-5.16448500	1.29011200	-0.03696400
C	-4.71221000	2.27369400	-0.92858700
C	-6.13932800	1.63351100	0.90796200
C	-5.21027100	3.57027000	-0.86313200
H	-3.96339700	2.01751200	-1.67115500
C	-6.64435600	2.92923100	0.95491500
H	-6.50749700	0.87892900	1.59522100
C	-6.18916700	3.93140400	0.08008100
H	-4.84366100	4.31355500	-1.56055900

H	-7.41569500	3.16760700	1.68087100
C	-3.28758900	-0.29484200	-0.17793400
C	-2.78956000	-1.45300100	-0.81486200
C	-2.35750500	0.60553200	0.38622200
C	-1.42925400	-1.69567700	-0.88186700
H	-3.48274300	-2.15399000	-1.26470400
C	-0.99768000	0.35759100	0.31018500
H	-2.71407700	1.49356400	0.89417800
C	-0.49775200	-0.79604100	-0.32381700
H	-1.05738100	-2.58235700	-1.38277200
H	-0.31519300	1.06676900	0.77055600
C	0.92330200	-1.08403600	-0.42307300
S	2.16015300	0.01157500	0.18772300
C	2.75849700	-2.20119100	-0.93036500
C	3.40153100	-1.10837500	-0.36423600
C	4.82768500	-0.88745300	-0.23763400
C	5.80181500	-1.60239400	-0.97413600
C	5.39145600	0.08561300	0.62913500
C	7.19501000	-1.37675400	-0.81489100
C	6.78996700	0.30437700	0.79637500
N	4.61155600	0.93901300	1.38539100
C	7.75648100	-0.43645700	0.08759700
N	7.97506300	-2.14892600	-1.65468700
C	9.19245500	-0.25345300	0.24459600
C	9.85749800	0.37129600	1.29969800
S	10.39096700	-0.78497200	-0.90847000
C	11.64792700	-0.09520900	0.11199800

C	13.02313600	-0.18774500	-0.29262200
H	13.23362900	-0.70139700	-1.22723200
C	14.11915500	0.29860200	0.35289300
C	14.09449700	1.01053900	1.58995900
C	15.44205500	0.05891900	-0.30444000
N	14.13752000	1.59722800	2.59389800
O	15.58539300	-0.52903200	-1.35711400
O	16.46671800	0.57053900	0.40441100
H	17.27495300	0.36745300	-0.09549100
H	3.26666900	-3.07934400	-1.30966900
H	9.36985200	0.75670000	2.18597300
N	-4.66430100	-0.04609400	-0.10567800
C	-6.70875500	5.31736800	0.20256900
C	-7.06012400	6.11325700	-0.91141500
C	-6.89093200	5.88876100	1.47251700
C	-7.56512600	7.41012400	-0.74735900
C	-7.38902500	7.17111300	1.65758900
H	-6.60820100	5.30556200	2.34351000
C	-7.72859600	7.93802200	0.53906700
H	-7.83217300	7.99747900	-1.61356500
H	-7.51132900	7.59690400	2.64694600
C	-8.47752900	-4.34723400	-0.08965200
C	-8.96492800	-4.98968300	1.07118600
C	-8.98288600	-4.79461500	-1.32123800
C	-9.90739700	-6.02344600	0.98790300
C	-9.91610900	-5.81682800	-1.42644800
H	-8.60809000	-4.33151900	-2.22885500

C	-10.38200400	-6.43625600	-0.26294100
H	-10.26958000	-6.49562500	1.88927100
H	-10.28496900	-6.15398800	-2.38840400
O	-8.20769100	9.18989300	0.79481800
O	-6.89808500	5.54285600	-2.14355000
O	-11.29465800	-7.43512500	-0.44094400
O	-8.48260000	-4.53545300	2.26729200
C	-8.56370600	10.01888000	-0.29939800
H	-8.91119100	10.95738900	0.13468300
H	-7.70461300	10.22121800	-0.95202000
H	-9.37257300	9.57836700	-0.89660500
C	-7.29809200	6.26439400	-3.29684700
H	-8.36760000	6.50869200	-3.27127200
H	-6.72045500	7.18952900	-3.42013100
H	-7.10151800	5.60560300	-4.14385800
C	-8.98457200	-5.09221800	3.47093400
H	-10.06796700	-4.94500100	3.56458000
H	-8.75872500	-6.16339900	3.55035800
H	-8.47988000	-4.56042400	4.27873700
C	-11.80107800	-8.10542700	0.70162400
H	-12.50070200	-8.85347500	0.32620800
H	-11.00396900	-8.60909200	1.26363300
H	-12.33471100	-7.41926000	1.37197900
S	6.97726000	1.61092700	1.92313100
S	5.61532800	-2.79825900	-2.21817500
N	7.35194100	-2.92115200	-2.43480400
N	5.22625800	1.77712500	2.09579300

N	1.40755700	-2.19006700	-0.96237800
N	11.20115000	0.45486600	1.22442600

Table S15: Cartesian coordinates of MS12 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*
C	-7.40436300	1.19747900	0.05391100
C	-7.05781300	2.27448600	-0.77573500
C	-8.50274300	1.33702900	0.91238500
C	-7.78016700	3.46182500	-0.73397200
H	-6.21429900	2.17745600	-1.45155700
C	-9.23056300	2.52273000	0.93436600
H	-8.79028400	0.50902400	1.55185800
C	-8.88547600	3.61685200	0.12173200
H	-7.49103300	4.27966100	-1.38286600
H	-10.09140600	2.59954100	1.59165700
C	-7.38924300	-1.25550700	-0.04499600
C	-7.04636900	-2.32863800	0.79114100
C	-8.46920400	-1.40731200	-0.92443500
C	-7.75426700	-3.52406000	0.73555100
H	-6.21684300	-2.22242700	1.48269900
C	-9.18306000	-2.60116600	-0.96026800
H	-8.75381200	-0.58254000	-1.56938200
C	-8.84123800	-3.69140800	-0.14111400
H	-7.46814400	-4.33874200	1.38970000
H	-10.03025100	-2.68757600	-1.63389800
C	-5.26443300	-0.01623800	0.02423500

C	-4.55083200	0.99377200	0.70123700
C	-4.52531100	-1.01790100	-0.63531300
C	-3.16527300	0.99931500	0.71145800
H	-5.09457200	1.76436400	1.23545600
C	-3.13891400	-1.00546000	-0.61646800
H	-5.04773400	-1.79872800	-1.17573600
C	-2.41760800	0.00297200	0.05146200
H	-2.65042700	1.77077400	1.27537100
H	-2.60448500	-1.77658000	-1.16403700
C	5.12609600	0.16614200	0.06084700
C	5.92865900	1.20718800	0.60192500
C	5.89385300	-0.86612400	-0.53044400
C	7.35316400	1.22730800	0.57467200
N	5.38055200	2.29799700	1.24784200
C	7.31499500	-0.84649300	-0.55346400
C	8.11303800	0.19600000	-0.01280900
N	7.86829200	-1.93922300	-1.19438200
C	15.61381200	0.45741200	0.02822200
H	16.02351800	1.45844600	0.14884100
C	16.57377000	-0.51370300	-0.07285400
C	16.27983400	-1.89781700	-0.23487200
C	17.99399200	-0.07717800	-0.00669900
N	16.00229200	-3.02172100	-0.36683300
O	18.35651300	1.07463200	0.12969400
O	18.85247400	-1.11375900	-0.11590600
H	19.74557900	-0.73501800	-0.06227700
N	-6.67017900	-0.02475100	0.01168200

C	-9.58872700	-4.96999200	-0.25387600
C	-9.99206800	-5.73195100	0.86617800
C	-9.94619700	-5.46499100	-1.51855900
C	-10.71331900	-6.92369900	0.71289200
C	-10.66018200	-6.64269800	-1.69316600
H	-9.62973700	-4.90887400	-2.39565800
C	-11.04644800	-7.37809100	-0.56881600
H	-11.01529700	-7.48607300	1.58418500
H	-10.91646700	-7.01199500	-2.67961300
C	-9.64938700	4.88690500	0.21998800
C	-10.04027800	5.64407800	-0.90769500
C	-10.03621700	5.37792500	1.47756200
C	-10.77783600	6.82753700	-0.76839300
C	-10.76673000	6.54743900	1.63832900
H	-9.73011800	4.82546100	2.36062800
C	-11.14015600	7.27825200	0.50667800
H	-11.06979700	7.38632000	-1.64539600
H	-11.04580300	6.91384500	2.61965800
O	-11.74108500	-8.52717200	-0.81440500
O	-9.65711000	-5.23379800	2.09490100
O	-11.85230600	8.41938000	0.73880700
O	-9.67654800	5.14968000	-2.12975600
C	-12.15489300	-9.31984700	0.28615900
H	-12.68010700	-10.17580700	-0.13990300
H	-11.29930200	-9.67894000	0.87267600
H	-12.83873600	-8.77199000	0.94741000
C	-10.09388500	-5.91530800	3.25890900

H	-11.18839900	-5.98115200	3.30345400
H	-9.66987000	-6.92569000	3.32374400
H	-9.73626400	-5.32368600	4.10283500
C	-10.10065700	5.82504900	-3.30199900
H	-11.19491100	5.87771300	-3.36605600
H	-9.68772500	6.84042000	-3.36024800
H	-9.72099600	5.23715700	-4.13887600
C	-12.25494900	9.20684100	-0.36961200
H	-12.79784300	10.05676400	0.04625300
H	-11.39293200	9.57570000	-0.94046000
H	-12.92007100	8.65086200	-1.04306000
C	3.67615500	0.16506300	0.11426600
C	2.83677000	-0.92252700	-0.10745500
C	1.47499700	-0.58106800	-0.04177900
C	1.23823900	0.76763700	0.22956800
C	-0.95917300	0.03101500	0.06794200
C	-0.13172400	1.11555000	0.29127800
H	3.18989700	-1.93175700	-0.26861700
H	-0.50495600	2.11823000	0.45577500
S	-0.02806200	-1.45374400	-0.20914600
S	2.72848700	1.63784500	0.44414700
C	14.19085300	0.34462400	-0.00192000
C	13.36344400	-0.76529100	-0.14823900
C	12.00313700	-0.41154000	-0.11078000
C	11.76412200	0.95902900	0.05529400
C	9.57067300	0.19706200	-0.06636800
C	10.39714800	1.30254400	0.07952300

H	13.74022200	-1.77169600	-0.27291000
H	10.03470400	2.31804100	0.15841500
S	10.51056600	-1.29567600	-0.27688100
S	13.25031800	1.84469000	0.17356400
S	7.86434300	2.66090200	1.41071200
S	5.38935000	-2.29909300	-1.37151200
N	6.19130700	3.13793300	1.71907600
N	7.05358000	-2.77699400	-1.66803300

Table S16: Cartesian coordinates of MS13 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(d, p) basis set.

Atom symbol	X	Y	Z
C	-7.24547900	-1.24449800	-0.00877600
C	-6.87899300	-2.27345800	0.87095500
C	-8.28651400	-1.47331000	-0.91715900
C	-7.52611400	-3.50349700	0.82932500
H	-6.07904700	-2.10609500	1.58495000
C	-8.94007100	-2.70152900	-0.93975000
H	-8.58868800	-0.68186500	-1.59508100
C	-8.57343100	-3.74914200	-0.07672800
H	-7.22316700	-4.28394500	1.51665500
H	-9.75914100	-2.84924400	-1.63699700
C	-7.39901000	1.20276900	0.04796500
C	-7.12551300	2.27102800	-0.81879500
C	-8.49808300	1.29939400	0.91053500
C	-7.92076000	3.41161100	-0.80859900
H	-6.28194000	2.20457300	-1.49829700

C	-9.29859700	2.43755300	0.90162500
H	-8.72903400	0.47496200	1.57704700
C	-9.02778500	3.52426500	0.05167200
H	-7.68816200	4.22462400	-1.48555300
H	-10.15868000	2.48142500	1.56282700
C	-5.19333600	0.11205500	0.06754700
C	-4.38797200	-0.88735000	-0.52163100
C	-4.54885300	1.20213600	0.69067400
C	-3.00779800	-0.79847600	-0.48682900
H	-4.85879200	-1.72909500	-1.01566200
C	-3.16680500	1.28645800	0.71614800
H	-5.14295500	1.97550000	1.16265800
C	-2.36117600	0.29211200	0.13067400
H	-2.40086700	-1.56655000	-0.95279600
H	-2.70934800	2.13463500	1.21814500
C	5.07118400	0.12587800	0.00411500
C	5.81863500	-0.70781200	-0.87027800
C	5.88924200	0.87749400	0.88000500
C	7.24115500	-0.78834000	-0.88896200
N	5.21427300	-1.50332400	-1.82470400
C	7.30844200	0.79898200	0.85849000
C	8.05255400	-0.03656500	-0.01523000
N	7.91581700	1.59678400	1.81031800
C	15.53353600	-0.55238800	-0.33347800
H	15.89723800	-1.47279000	-0.78631100
C	16.53625200	0.29471100	0.05558900
C	16.30539700	1.55864000	0.67014900

C	17.93521000	-0.14873300	-0.18681600
N	16.07910400	2.58625300	1.17051900
O	18.24495000	-1.20439100	-0.70274900
O	18.83942800	0.76143200	0.23409200
H	19.71448300	0.38845400	0.03625000
N	-6.59187500	0.02467100	0.03546500
C	-9.86948800	4.74634100	0.11590300
C	-10.31295400	5.44161600	-1.03204800
C	-10.27957800	5.25138900	1.36052500
C	-11.12252500	6.58040200	-0.92414100
C	-11.08076600	6.37755500	1.49014700
H	-9.93471800	4.74732100	2.25813400
C	-11.50532000	7.04762700	0.33896500
H	-11.45379500	7.09186500	-1.81591100
H	-11.37683500	6.75671500	2.46158100
C	-9.25438300	-5.06551400	-0.17422100
C	-9.65649600	-5.81426500	0.95513800
C	-9.54611700	-5.61295600	-1.43420000
C	-10.31421600	-7.04375900	0.81508900
C	-10.19618600	-6.82879900	-1.59560800
H	-9.22813900	-5.06729100	-2.31727600
C	-10.58310000	-7.55006200	-0.46225700
H	-10.61697200	-7.59545900	1.69290700
H	-10.40177900	-7.23825200	-2.57804200
O	-12.28596800	8.14866400	0.54080300
O	-9.92555800	4.93258200	-2.24055400
O	-11.21324700	-8.73804200	-0.69496100

O	-9.38607900	-5.26560400	2.17813600
C	-12.74280900	8.87488800	-0.58840900
H	-13.33506100	9.70209700	-0.19477200
H	-11.90839900	9.27833800	-1.17654500
H	-13.37585600	8.25807900	-1.23938900
C	-10.39676000	5.54315500	-3.43045500
H	-11.49241700	5.52509400	-3.48867700
H	-10.04851300	6.57997300	-3.52268500
H	-9.98486700	4.95421600	-4.25116100
C	-9.82452400	-5.93594700	3.34813700
H	-10.91533100	-6.05496200	3.36238500
H	-9.35359300	-6.92169100	3.45441000
H	-9.52242200	-5.30429100	4.18470000
C	-11.62395900	-9.51905300	0.41519300
H	-12.09330600	-10.41122200	-0.00163800
H	-10.77153000	-9.81928800	1.03820800
H	-12.35444000	-8.98703700	1.03838300
C	3.62076500	0.20047100	-0.00477600
C	2.84375500	1.21815200	0.54336600
C	1.46637100	0.96285100	0.43316200
C	1.16921700	-0.24584400	-0.19557800
C	-0.90969700	0.35227400	0.14004700
H	3.25498100	2.12573000	0.96315400
S	-0.03064100	1.74994300	0.85388200
S	2.60619100	-1.08391500	-0.70383400
C	14.11718800	-0.40225200	-0.23113200
C	13.34149800	0.62831200	0.29220600

C	11.96648000	0.35786300	0.17610600
C	11.66545400	-0.87203000	-0.42374200
C	9.50948900	-0.11017800	-0.00270900
C	10.28442700	-1.13667500	-0.52411000
H	13.76366700	1.52297500	0.73002900
H	9.87656100	-2.05526500	-0.92245700
S	10.51654500	1.19390400	0.66120600
S	13.10967400	-1.72488700	-0.86412400
S	7.67846100	-1.88387000	-2.16323700
S	5.45587600	1.96814100	2.16002600
N	5.98178600	-2.16986600	-2.56680700
N	7.14325800	2.25914300	2.55488000
N	-0.12972600	-0.58248000	-0.35999000

Table S17: Cartesian coordinates of MS14 dye in the singlet closed-shell ground-state, optimized with B3LYP functional and 6-31G(*d, p*) basis set.

Atom symbol	*X*	*Y*	*Z*
C	-7.23491500	-1.21853800	-0.00454600
C	-6.87801400	-2.25076900	0.87527000
C	-8.27969800	-1.43672400	-0.91120200
C	-7.53820600	-3.47389900	0.83533000
H	-6.07529800	-2.09145500	1.58800200
C	-8.94624400	-2.65797400	-0.93213200
H	-8.57450900	-0.64245600	-1.58906700
C	-8.58940800	-3.70892600	-0.06904900
H	-7.24256100	-4.25711700	1.52268400
H	-9.76791500	-2.79738300	-1.62801900

C	-7.36300900	1.23013000	0.05269700
C	-7.08173700	2.29495700	-0.81575900
C	-8.45798100	1.33832400	0.91905000
C	-7.86530700	3.44357700	-0.80345900
H	-6.24131400	2.21950300	-1.49822400
C	-9.24689800	2.48456800	0.91228400
H	-8.69493400	0.51663700	1.58684800
C	-8.96803500	3.56798900	0.06071700
H	-7.62688100	4.25378300	-1.48173600
H	-10.10416100	2.53755900	1.57646300
C	-5.16871100	0.11669300	0.06676600
C	-4.37503400	-0.89226500	-0.52222400
C	-4.51143200	1.20135400	0.68622000
C	-2.99401100	-0.81762000	-0.49078000
H	-4.85566300	-1.73002900	-1.01353900
C	-3.12861300	1.27133200	0.70840700
H	-5.09634300	1.98173900	1.15809200
C	-2.33463900	0.26747800	0.12305700
H	-2.39616900	-1.59285200	-0.95663800
H	-2.66124100	2.11562900	1.20780000
C	5.09468900	0.02375000	-0.01993900
C	5.83077800	-0.82578500	-0.88893200
C	5.92338900	0.77534300	0.84670100
C	7.25233500	-0.92034000	-0.91176500
N	5.21581500	-1.62380500	-1.83438000
C	7.34150600	0.68308700	0.82036400
C	8.07350600	-0.16712500	-0.04917400

N	7.96094200	1.48221700	1.76347900
C	15.47070900	-0.46015300	-0.27278300
H	15.94679300	-1.35323500	-0.66919900
C	16.33243700	0.51741300	0.12760900
C	15.94386300	1.77615800	0.67511800
C	17.79042600	0.22575800	-0.03081900
N	15.68000600	2.81664000	1.12459200
O	18.23496800	-0.80914000	-0.48537700
O	18.56546600	1.24431500	0.38880600
H	19.48569800	0.96549000	0.24820300
N	-6.56790900	0.04378100	0.03806700
C	-9.79693700	4.79864300	0.12727200
C	-10.23709700	5.49802900	-1.01945700
C	-10.19753500	5.30835600	1.37309400
C	-11.03447800	6.64515800	-0.90924400
C	-10.98656300	6.44279300	1.50498500
H	-9.85481200	4.80112600	2.26974000
C	-11.40808900	7.11680100	0.35497300
H	-11.36348000	7.15969800	-1.80008200
H	-11.27534000	6.82538700	2.47726600
C	-9.28440400	-5.01805800	-0.16474000
C	-9.69265600	-5.76187300	0.96568200
C	-9.58385800	-5.56307600	-1.42396400
C	-10.36352900	-6.98442900	0.82734600
C	-10.24695800	-6.77207700	-1.58366700
H	-9.26151700	-5.02129300	-2.30784900
C	-10.63970000	-7.48859000	-0.44929600

H	-10.67074200	-7.53240200	1.70594700
H	-10.45838600	-7.17989000	-2.56554300
O	-12.17657100	8.22591200	0.55902100
O	-9.85912400	4.98456500	-2.22906300
O	-11.28266500	-8.66998000	-0.68033400
O	-9.41458900	-5.21540700	2.18793200
C	-12.62946600	8.95664300	-0.56889600
H	-13.21164200	9.79014900	-0.17352500
H	-11.79278500	9.35110700	-1.15988400
H	-13.27114400	8.34638000	-1.21758500
C	-10.32785500	5.59970300	-3.41761200
H	-11.42382500	5.59308700	-3.47219300
H	-9.96907500	6.63278500	-3.51131000
H	-9.92486700	5.00624700	-4.23948200
C	-9.85847800	-5.88031500	3.35900600
H	-10.95045800	-5.98777900	3.37482000
H	-9.39783600	-6.87090500	3.46528500
H	-9.54856000	-5.25133200	4.19472000
C	-11.69973700	-9.44608800	0.43090500
H	-12.17904200	-10.33351800	0.01529700
H	-10.84947800	-9.75487100	1.05270100
H	-12.42361900	-8.90614100	1.05496500
C	3.64543700	0.11290000	-0.02531600
C	2.87997700	1.14056700	0.52107800
C	1.50004300	0.89942700	0.41467800
C	1.18887200	-0.30830600	-0.20953300
C	-0.88282300	0.31261100	0.12901200

H	3.30131500	2.04519900	0.93711800
S	0.01227300	1.70344100	0.83618200
S	2.61574300	-1.16321000	-0.71800800
C	14.03902600	-0.44666500	-0.23217300
C	11.97994800	0.19358500	0.09224600
C	11.66909000	-1.05870100	-0.45792300
C	9.53008900	-0.25455500	-0.04316900
C	10.28569400	-1.31217900	-0.53435200
H	9.85891400	-2.23873200	-0.89178700
S	10.54844000	1.06876900	0.56285900
S	13.14453200	-1.87456500	-0.84766700
S	7.67545900	-2.03137200	-2.17745600
S	5.50597400	1.88050300	2.11943600
N	5.97408100	-2.30436200	-2.57308900
N	7.19775100	2.15792100	2.50549900
N	-0.11367800	-0.63196800	-0.36981900
N	13.27494700	0.52702200	0.21972300

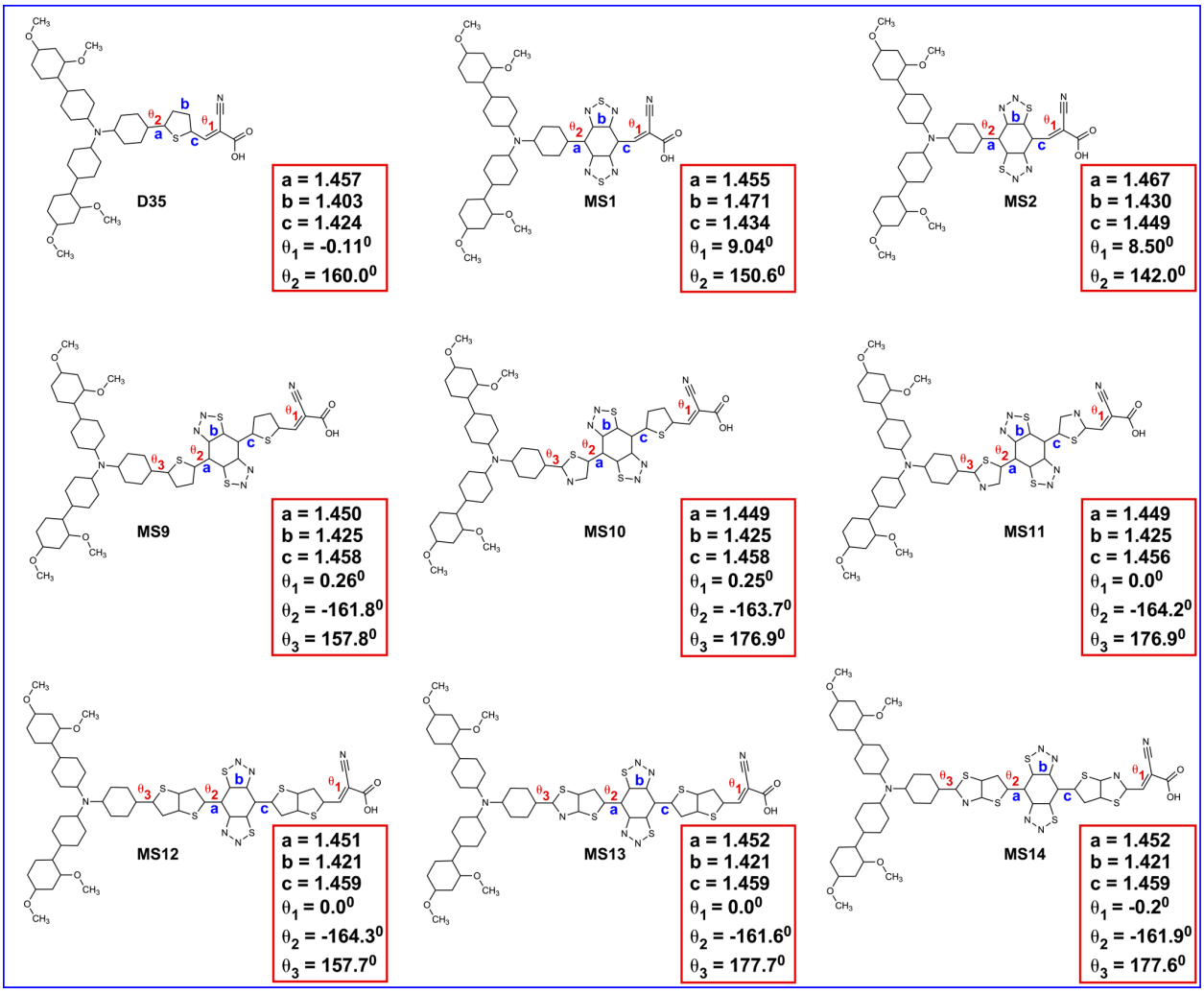

Figure S1: Bond lengths (Å) and dihedral angles (θ) of the closed-shell reference and designed dyes.

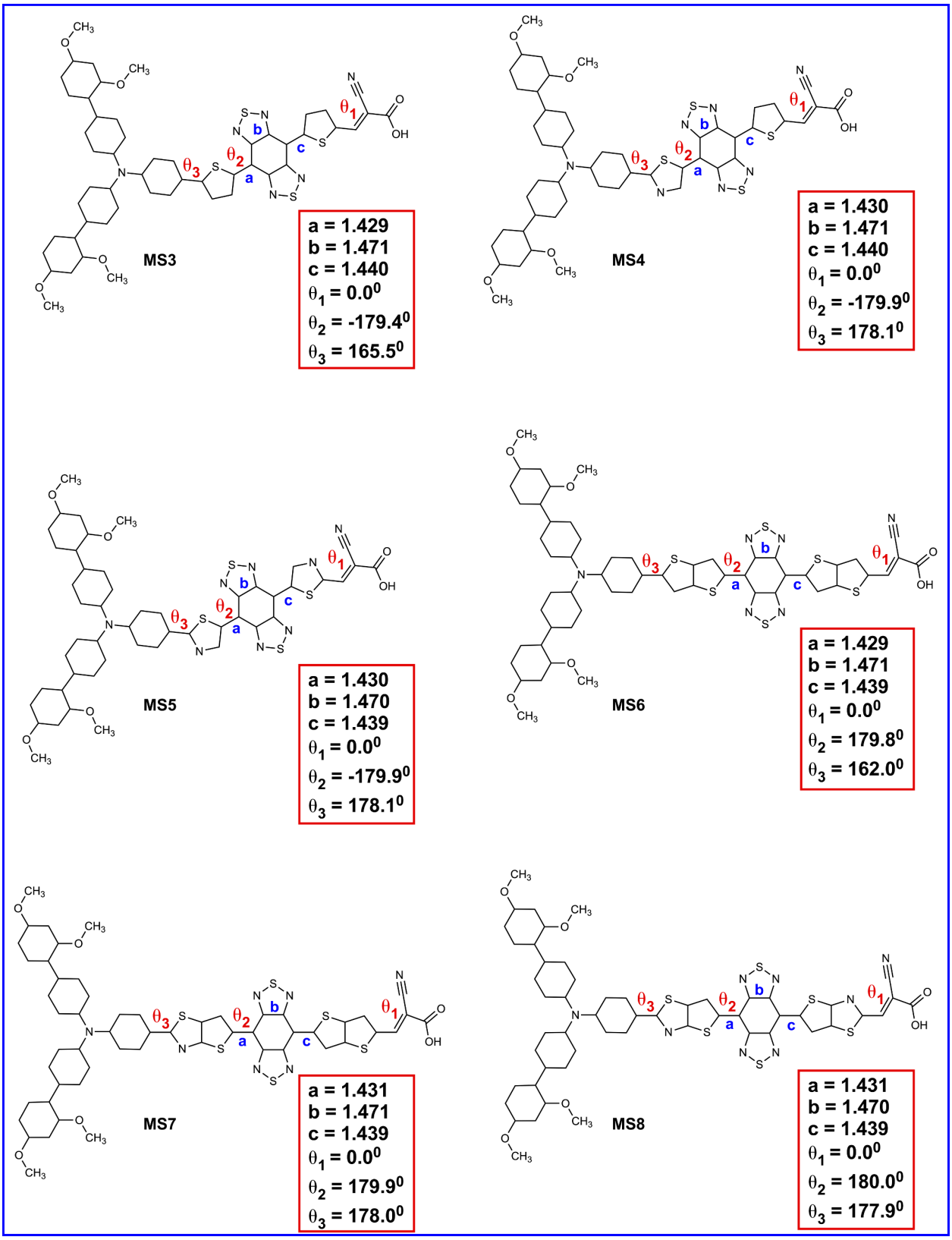

Figure S2: Bond lengths (Å) and dihedral angles (θ) of the open-shell dyes.

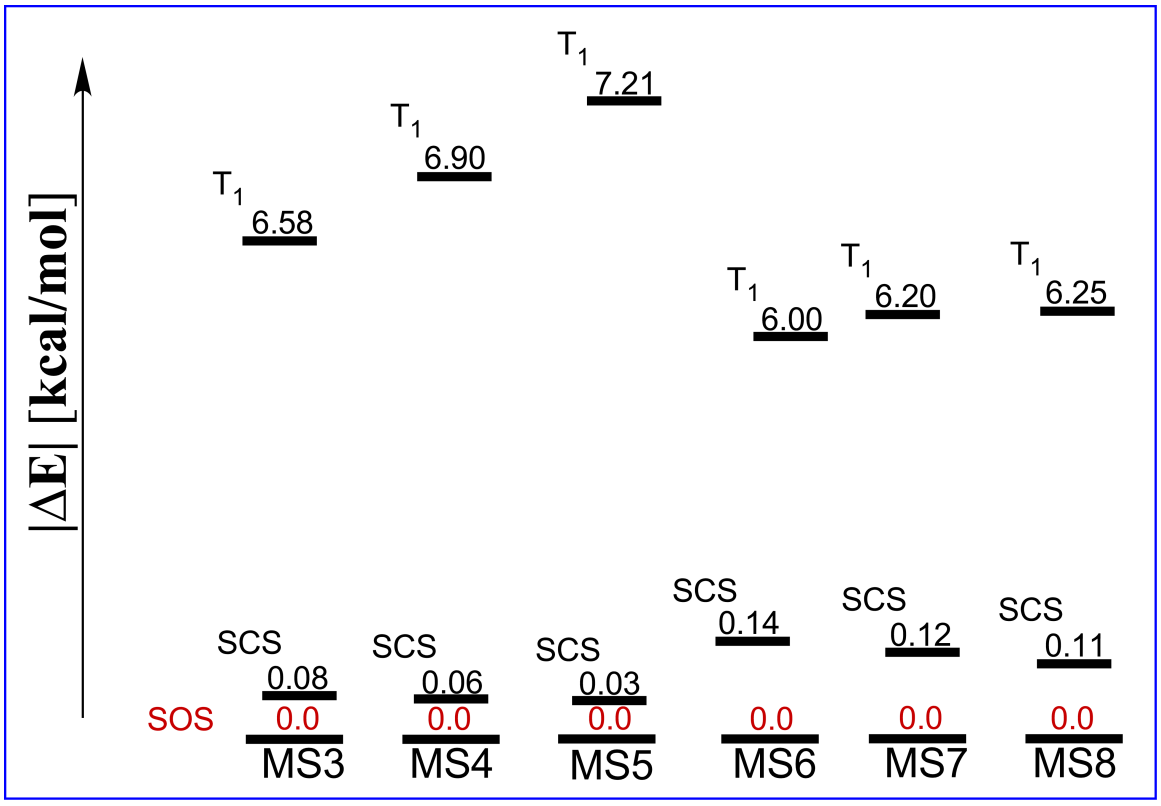

Figure S3: Energy diagram of the open-shell dyes. Energy values are calculated with reference to the singlet open-shell (SOS) configuration. SCS = singlet closed-shell, and T1 is the lowest triplet state.

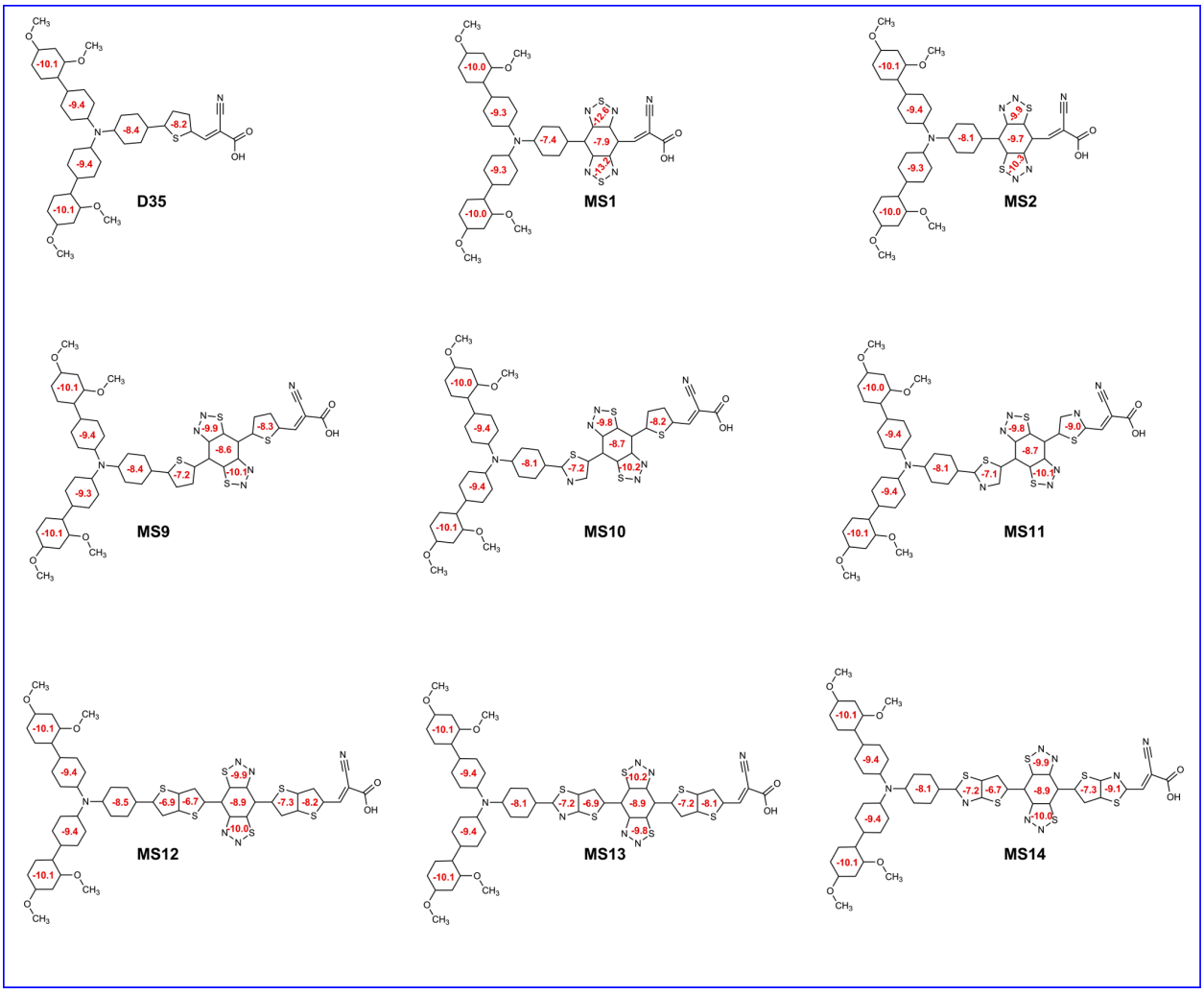

Figure S4: Calculated $NICS_{iso}(1)$ values of the closed-shell dyes.

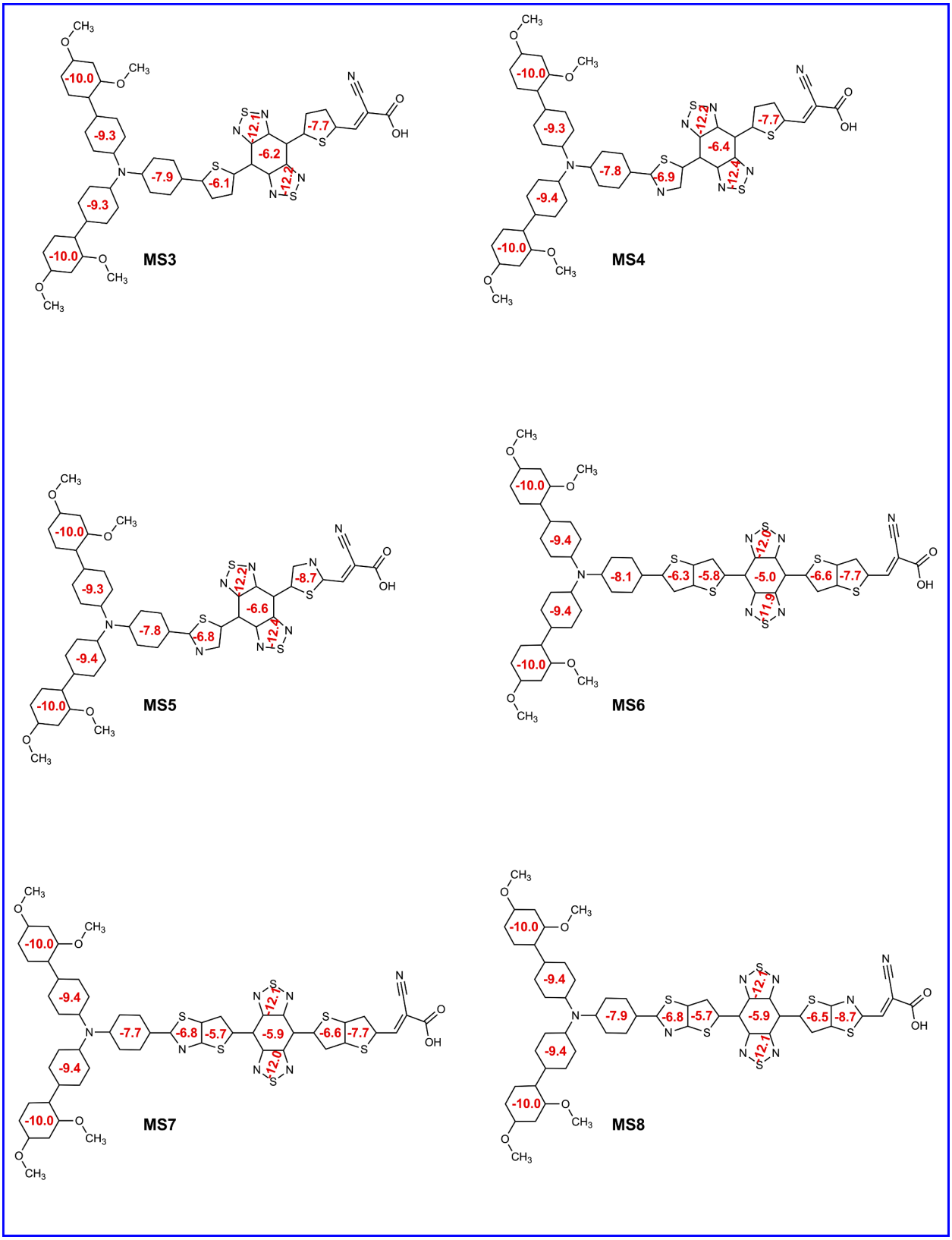

Figure S5: Calculated NICS$_{iso}$(1) values of the open-shell dyes.

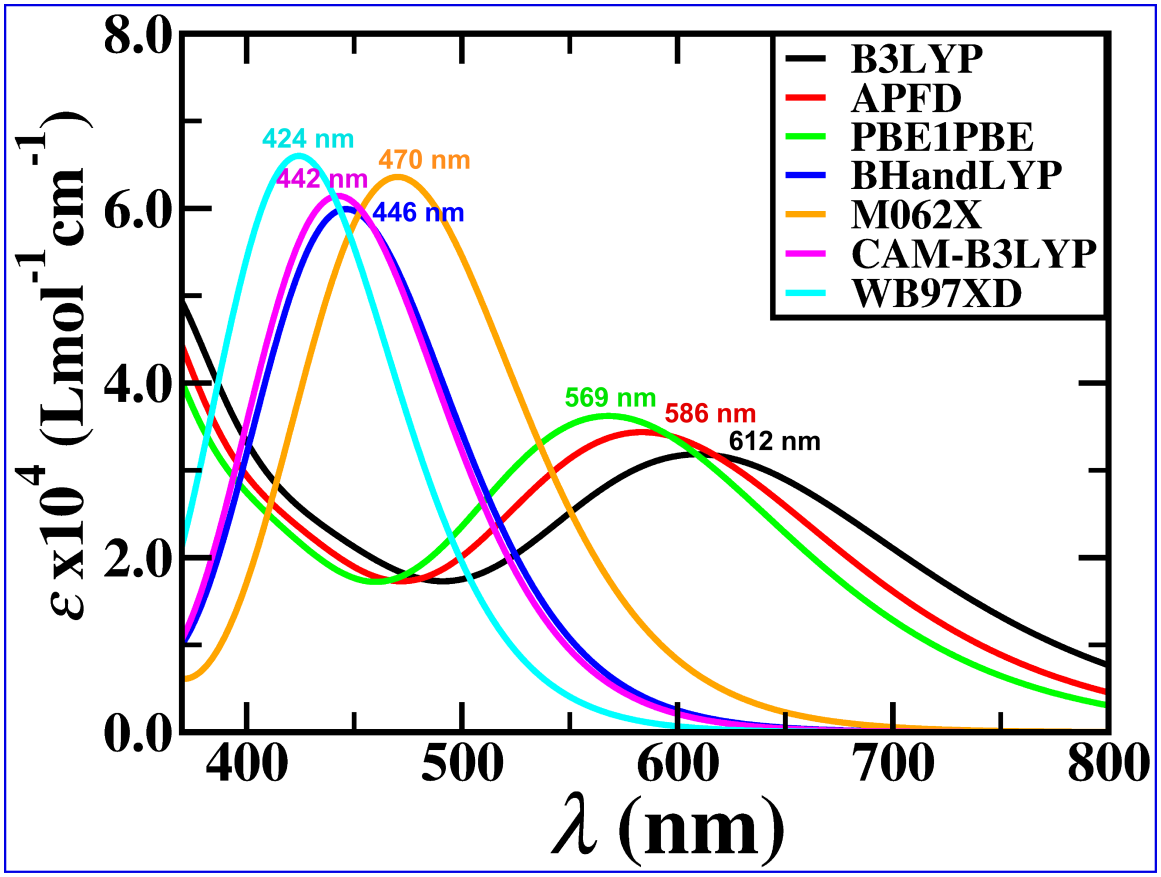

Figure S6: Benchmark absorption calculation on the parent dye (D35) at different density functionals. The density functionals used with increasing percentage of HF exchange in ethanol implicit solvent.

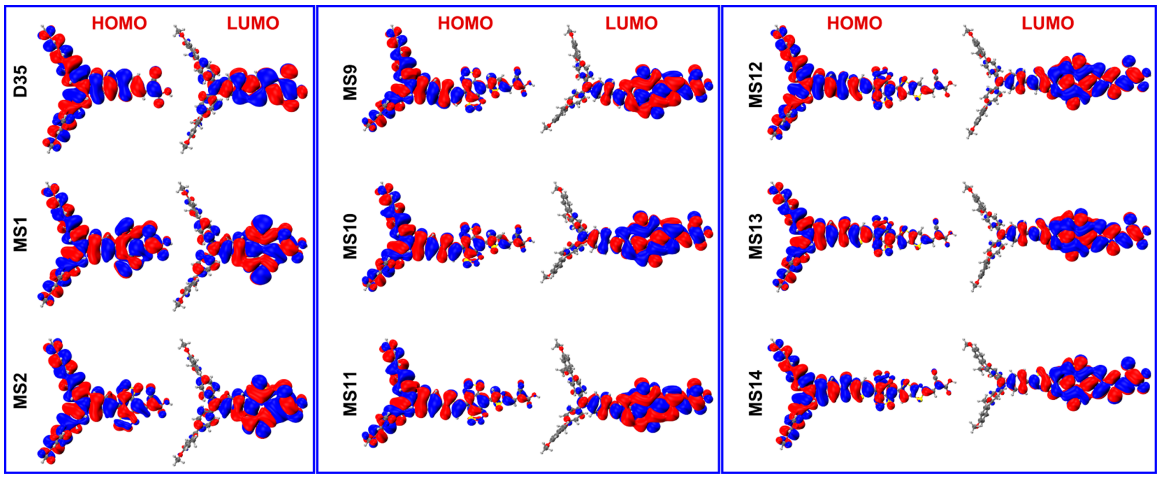

Figure S7: Molecular orbital (MO) diagrams of the closed-shell dyes. The red and blue surface represents the positive and negative contribution on the wave function, respectively, at an isovalue = 0.005 au.

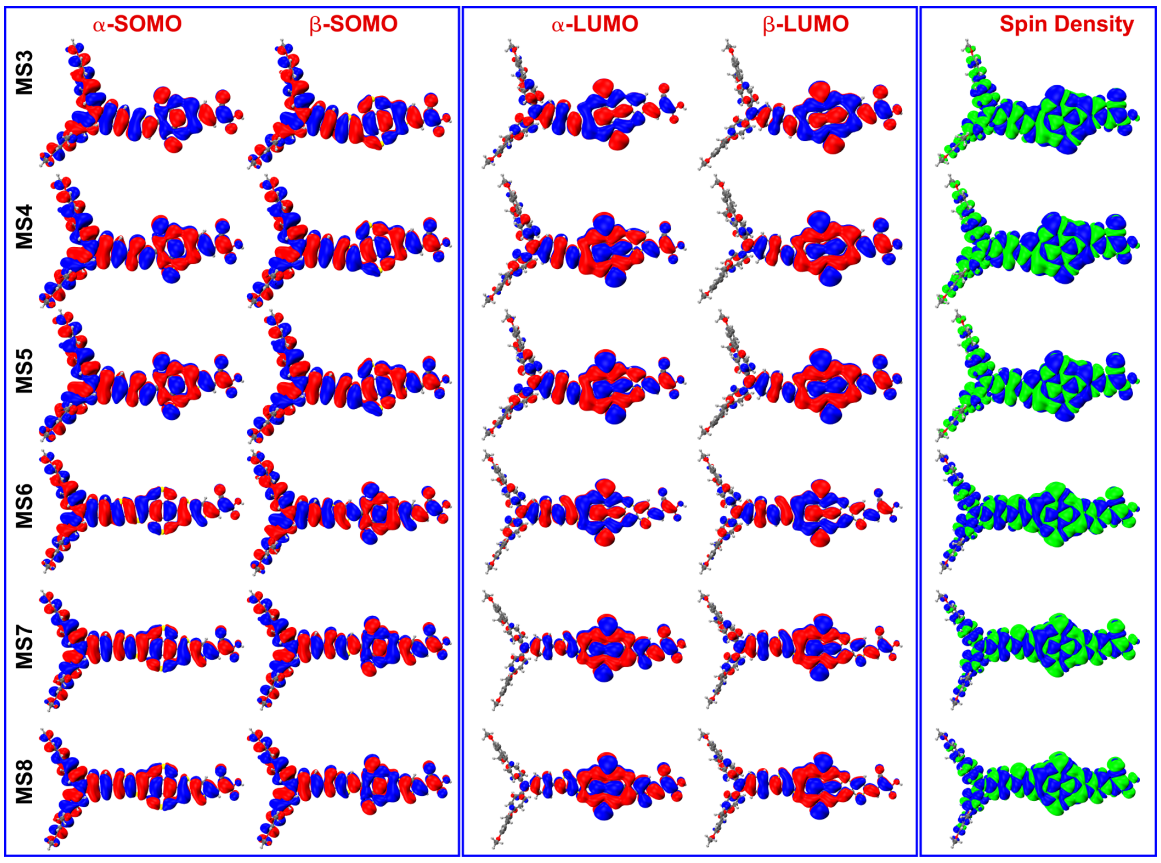

Figure S8: Molecular orbital (MO) diagrams and spin density distributions of the open-shell dyes. For MO diagram, the red and blue surface represents the positive and negative contribution on the wave function, respectively, at an isovalue = 0.005 au. In the spin density distributions, the blue and green surfaces represents the positive and negative spin contribution, respectively, at a isovalue = 9×10^{-6} au.