

Supporting information

**Photoactive layer based on T-shaped benzimidazole dyes
used for solar cell: from photoelectric properties to
molecular design**

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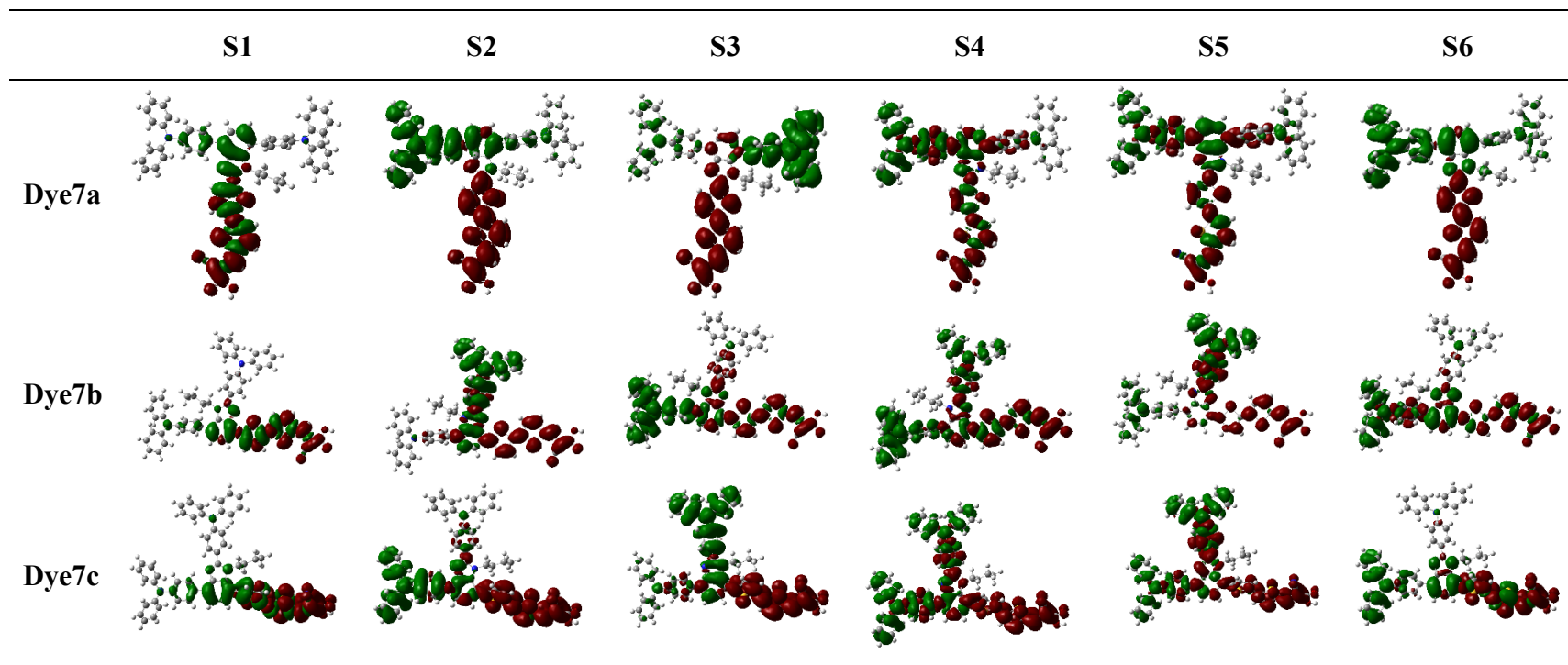


Figure S1. Electron density difference plots electronic transition for isolated dyes.

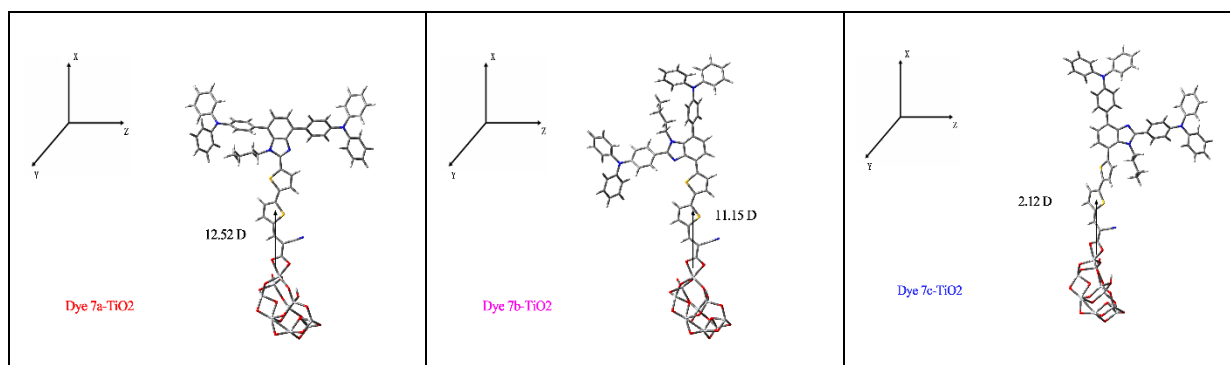


Figure S2. Calculated vertical dipole moment on TiO₂ surface.

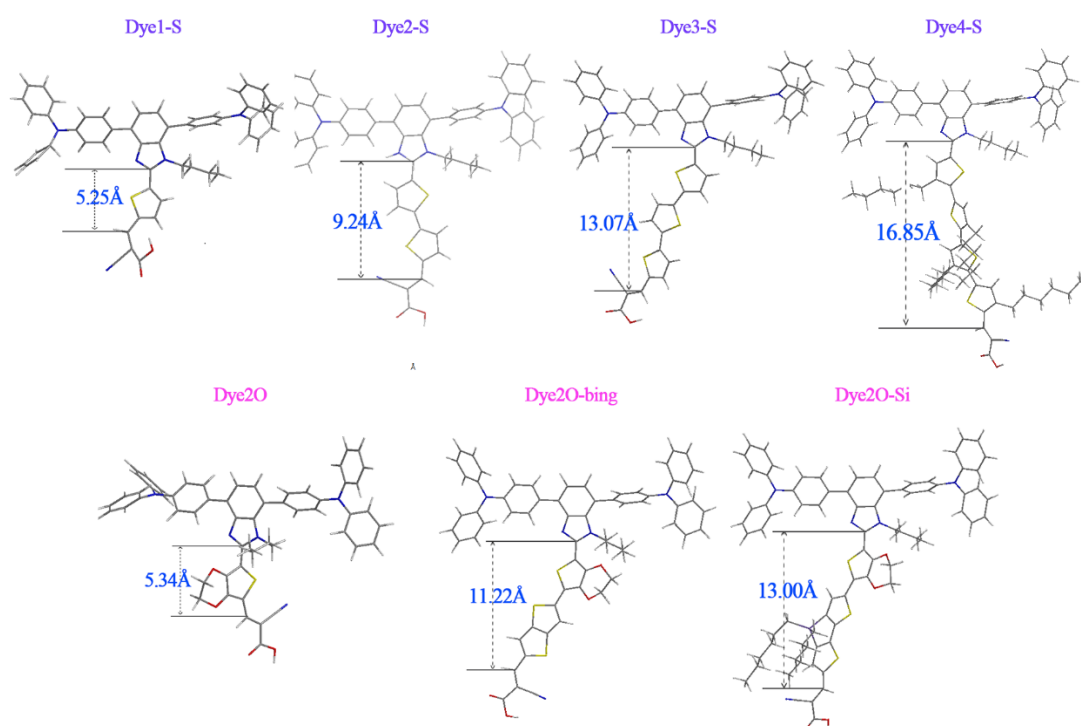


Figure S3. The lengths of π spacers obtained from the optimized designed dyes.

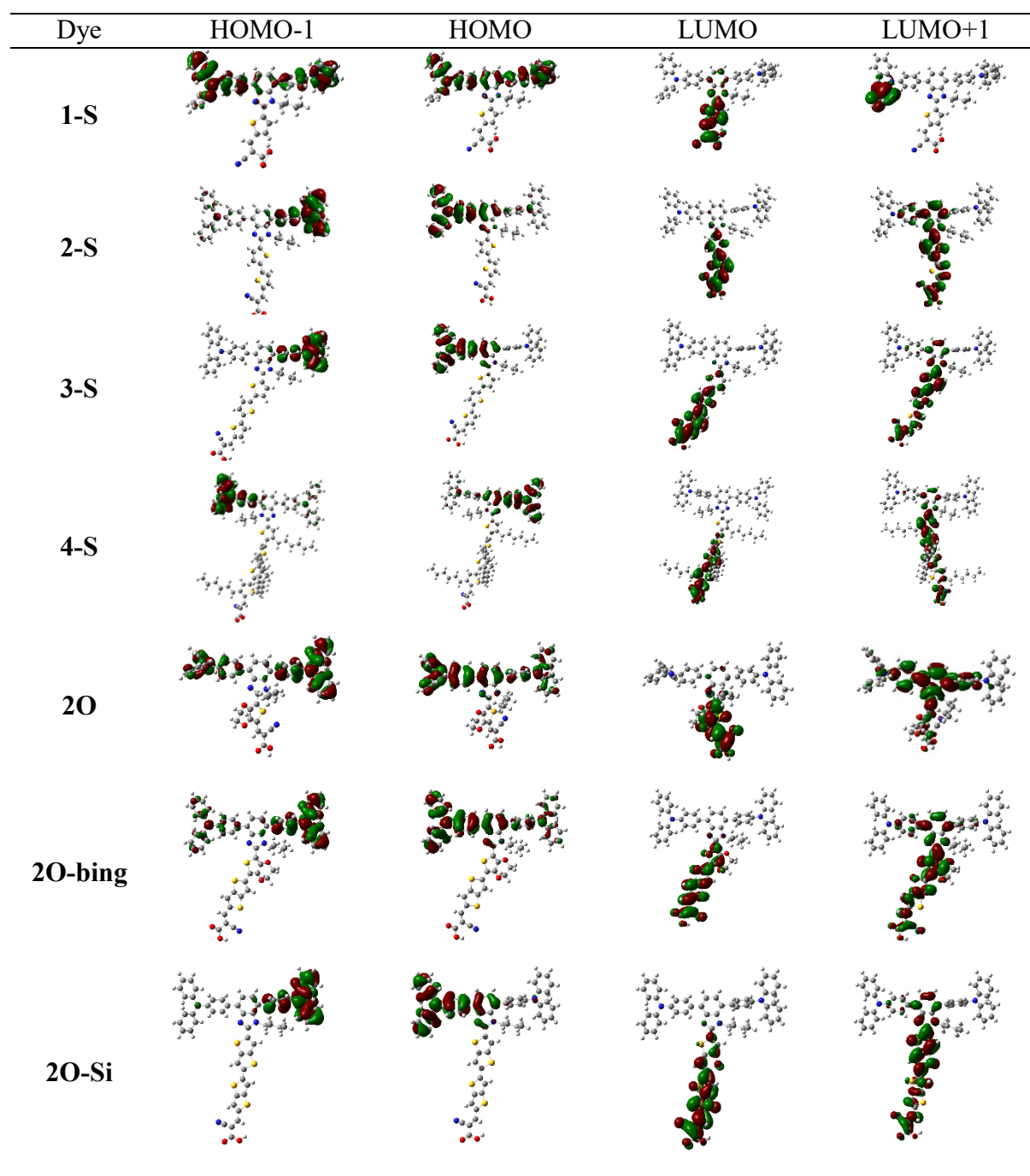


Figure S4. The frontier molecular orbitals for designed dyes.

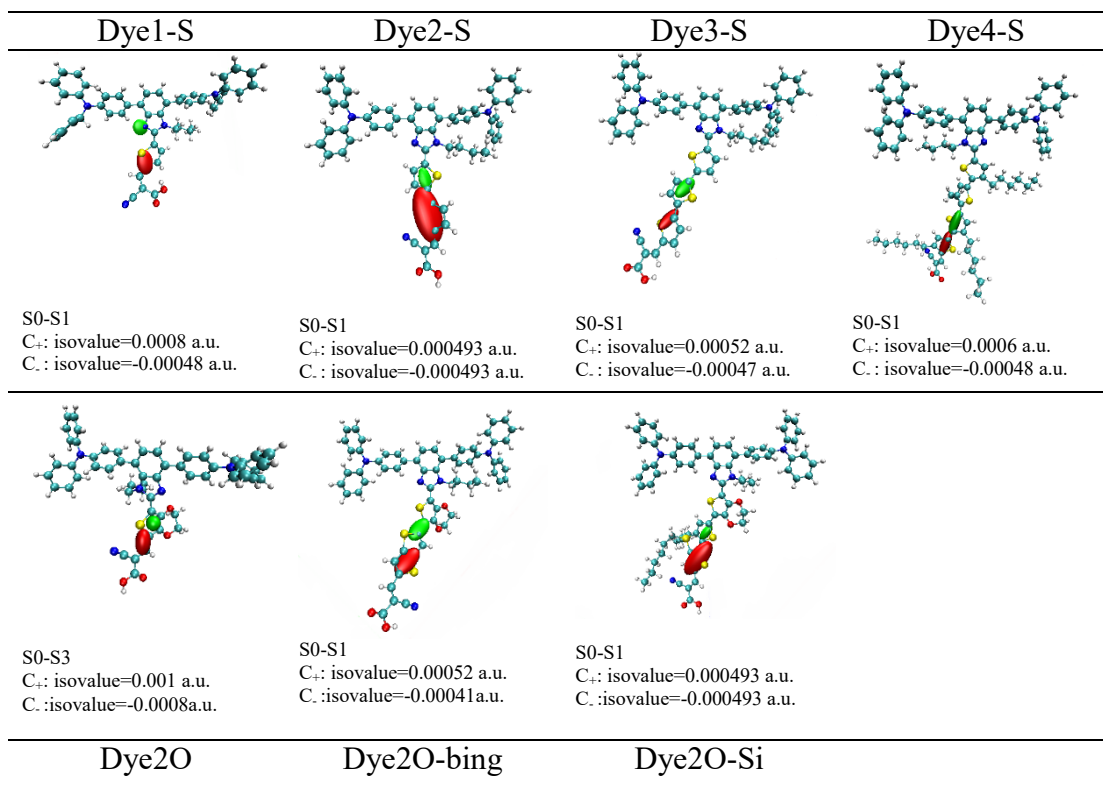


Figure S5. Computed difference in the centroids of hole and charge (C₊/C₋).

Table S1. Maximum absorption wavelength (λ_{\max}) data using different methods.

	B3LYP	CAM-B3LYP	ω B97xD	Exp[a]
Dye7a	519.01	451.31	439.55	428
Dye7b	515.27	473.44	461.01	469
Dye7c	475.53	423.97	404.83	418

Data [a] was taken from Ref¹

Table S2. Transition electric dipole moments.

		X	Y	Z
7a	S1	-1.6494	-4.5178	-0.0229
	S2	1.9211	0.0452	-0.0245
	S3	0.0871	-0.0307	-0.0369
	S4	-2.4930	1.3851	0.0568
	S5	2.0791	-0.3125	0.1151
	S6	0.0833	0.2291	-0.0125
7b	S1	4.9722	1.2553	0.0544
	S2	1.1159	1.7423	-0.0108
	S3	1.2000	0.3957	0.0878
	S4	-0.0723	1.1073	0.0054
	S5	-1.3643	-2.2991	0.0044
	S6	1.6566	-0.2189	0.0825
7c	S1	4.7610	-0.3690	0.1188
	S2	0.6508	-1.3187	-0.0789
	S3	0.6036	1.3460	-0.0213
	S4	1.5259	-2.2827	0.0432
	S5	2.2113	1.7315	0.0558
	S6	-0.3717	0.1594	-0.2191

Table S3. The distances of I-X (X=I, N and S) for isolated dyes.

Dyes...I ₂	CN...I1	I1...I2	S _{thiophene1} ...I3	I3...I4	S _{thiophene2} ...I5	I5...I6
7a	2.700	2.877	3.352	2.858	3.295	2.864
7b	2.670	2.882	3.305	2.864	3.160	2.886
7c	2.690	2.879	3.337	2.860	3.329	2.862

Table S4. Cartesian coordinates and total energies

Dye 7a (total energy= -3494.49877308 a.u)			
C	0.33420100	0.29858400	-0.07668600
N	1.10280800	-0.77700500	-0.09632200
N	-1.02005400	-0.01286500	-0.06780100
C	0.25121300	-1.85207600	-0.07991000
C	-1.09996000	-1.40623400	-0.07235700
C	0.58381300	-3.23076500	-0.06329500
C	-2.18751600	-2.30628400	-0.06615600
C	-0.50377700	-4.10702600	-0.01801000
C	-1.83229100	-3.65881500	-0.02158100
H	-0.31997400	-5.17542900	0.03824900
H	-2.63261000	-4.39349300	-0.00381700
C	-2.14155800	0.91586400	0.08581900
C	-2.52444900	1.16769600	1.55054700
H	-2.99308000	0.50343400	-0.45543400
H	-1.87920600	1.84989600	-0.41790400
C	-3.71599000	2.12457400	1.68008800
H	-2.76977900	0.20651600	2.01912000
H	-1.65971200	1.57227600	2.09283100
C	-4.11202900	2.38693000	3.13651900
H	-3.47586600	3.07781700	1.18764600
H	-4.57459800	1.70468200	1.13727800
H	-4.96474800	3.07207000	3.19947100
H	-4.39397300	1.45602000	3.64266400
H	-3.28270700	2.83260400	3.69885100
C	-3.63562300	-1.94871800	-0.12429800
C	-4.47896700	-2.18029000	0.97327500
C	-4.22299500	-1.45436200	-1.30119300
C	-5.84316600	-1.90541200	0.91323800
H	-4.05421800	-2.56774000	1.89565200
C	-5.58787100	-1.19300900	-1.37842600
H	-3.60338000	-1.30103900	-2.18140900
C	-6.42170900	-1.40996800	-0.26739600
H	-6.46800200	-2.07756500	1.78352900
H	-6.01779800	-0.83105600	-2.30662700
N	-7.81126200	-1.14440800	-0.33942300
C	-8.73953700	-2.00329600	0.31629700
C	-8.29385500	-0.02996500	-1.08175000
C	-9.81077500	-1.46375900	1.04525800
C	-8.60088900	-3.39803700	0.23837000
C	-9.41457700	-0.16407700	-1.91662100
C	-7.66361300	1.22089700	-0.98500700
C	-10.72577000	-2.30523300	1.67545400
H	-9.92030800	-0.38589800	1.11178500
C	-9.51015500	-4.23141900	0.88739100
H	-7.77973500	-3.82171700	-0.33124400
C	-9.89441200	0.93219400	-2.63090300

H	-9.90440200	-1.12907900	-1.99954300
C	-8.13942800	2.30708600	-1.71707300
H	-6.80318700	1.33550500	-0.33284800
C	-10.57953000	-3.69224200	1.60569100
H	-11.54995700	-1.87146800	2.23564300
H	-9.38846200	-5.30914300	0.81723700
C	-9.25888000	2.17238100	-2.54091900
H	-10.76323800	0.81012300	-3.27233500
H	-7.63954500	3.26830100	-1.62966700
H	-11.29047400	-4.34487700	2.10419500
H	-9.63156400	3.02282500	-3.10453200
C	1.97512300	-3.73242200	-0.09021800
C	2.28111800	-4.95328200	-0.72024100
C	3.03615500	-3.04206000	0.52484600
C	3.57279600	-5.46504200	-0.73538100
H	1.49979800	-5.49505600	-1.24575900
C	4.32777200	-3.55603200	0.52966600
H	2.83954500	-2.09692400	1.01587000
C	4.62006500	-4.77623700	-0.10154800
H	3.77970100	-6.39801500	-1.24975900
H	5.12158000	-3.01213700	1.03180300
N	5.93954700	-5.29707200	-0.10592200
C	6.15521200	-6.69194600	0.06501400
C	7.05010700	-4.42655100	-0.28677400
C	7.10468000	-7.36877300	-0.71776000
C	5.42313500	-7.41494100	1.02107000
C	8.20938700	-4.58047000	0.49038200
C	7.00469900	-3.40212500	-1.24606700
C	7.31917700	-8.73411600	-0.53912300
H	7.67029300	-6.81878300	-1.46316200
C	5.63198700	-8.78352700	1.17961400
H	4.69318500	-6.89776600	1.63571300
C	9.29954800	-3.73302000	0.30200200
H	8.24829400	-5.36574700	1.23863800
C	8.09310900	-2.54826600	-1.41445100
H	6.11414900	-3.28126900	-1.85456200
C	6.58286600	-9.45215400	0.40562900
H	8.05816000	-9.24095100	-1.15439000
H	5.05628900	-9.32621600	1.92502700
C	9.24858300	-2.70963700	-0.64683800
H	10.18873900	-3.86638100	0.91276600
H	8.04065500	-1.76058400	-2.16160300
H	6.74815100	-10.51770400	0.53717400
H	10.09741600	-2.04617900	-0.78558600
C	0.95009000	1.61854300	-0.10255200
C	2.29859500	1.80915900	-0.35334300
S	0.17954600	3.15665400	0.23160800
C	2.70670800	3.15516000	-0.29082600
H	2.95140200	0.97444700	-0.57393500
C	1.68321500	4.03591700	0.01458600

H	3.72713200	3.47709600	-0.47057200
C	1.72797400	5.46839200	0.15010200
C	0.68378700	6.34256300	0.43466100
S	3.23510400	6.33546900	-0.04463300
C	1.08800600	7.68336300	0.49359600
H	-0.33761800	6.01403100	0.59191000
C	2.44658700	7.88040300	0.25775700
H	0.41579100	8.50935800	0.70240100
C	3.07291200	9.15981700	0.26676300
C	4.37806800	9.52071200	0.05488000
H	2.39175500	9.97993200	0.47770800
C	5.40735500	8.57611000	-0.23544700
C	4.81580600	10.93519000	0.11242300
N	6.22632800	7.78231100	-0.47113000
O	5.95440900	11.31301400	-0.06632500
O	3.79690700	11.79385100	0.39119400
H	4.20247900	12.68002900	0.40247500

Dye 7b(total energy= -3494.50524186 a.u)

C	-0.11630700	0.55352900	0.08023700
N	0.78582500	-0.40893700	0.01936300
N	-1.41558700	0.05959000	0.09543900
C	0.08367000	-1.58594800	0.01147600
C	-1.31282800	-1.33308500	0.04071300
C	0.61566000	-2.89559200	0.01044900
C	-2.25586400	-2.38290600	0.02981100
C	-0.33137000	-3.93001500	0.05007100
C	-1.70437500	-3.67424600	0.05582700
H	-0.00299400	-4.96368700	0.06512400
H	-2.39040700	-4.51640000	0.04935500
C	-2.64404200	0.85475300	0.14834200
C	-3.30370900	0.88577200	1.53335300
H	-3.34696100	0.45237700	-0.58369600
H	-2.38496700	1.86497300	-0.17626700
C	-4.54107900	1.79214800	1.55652200
H	-3.58720300	-0.13389000	1.81871900
H	-2.57557900	1.22665200	2.28181800
C	-5.24511600	1.80288700	2.91723400
H	-4.24995900	2.81696800	1.28459900
H	-5.24534800	1.45919600	0.78119900
H	-6.11989000	2.46266800	2.90831400
H	-5.58637000	0.79785600	3.19226400
H	-4.57191500	2.15295600	3.70914400
C	0.26856600	1.97476700	0.07714200
C	-0.33830000	2.96624900	0.86646800

C	1.36286300	2.35638700	-0.72113100
C	0.11160500	4.28182600	0.84575100
H	-1.13943800	2.70827500	1.55069500
C	1.80800000	3.66976700	-0.75868600
H	1.85231300	1.60174600	-1.32770100
C	1.18659700	4.66180100	0.02358000
H	-0.36103800	5.02074700	1.48390900
H	2.63886200	3.93813800	-1.40242500
N	1.63511600	5.99999900	-0.00975400
C	0.71086300	7.07569300	0.12949900
C	3.02012800	6.29402800	-0.17664500
C	1.00481000	8.15659100	0.97465700
C	-0.49709400	7.07573500	-0.58540900
C	3.42668900	7.29459200	-1.07228300
C	3.99170300	5.59776000	0.55873500
C	0.10740800	9.21612900	1.09666600
H	1.93728700	8.16010400	1.53024300
C	-1.39646900	8.13092400	-0.44342600
H	-0.72278300	6.24811100	-1.25061300
C	4.77953600	7.59425700	-1.22238800
H	2.67818700	7.83264400	-1.64543000
C	5.34350400	5.89197700	0.38879100
H	3.68187100	4.82919500	1.26002800
C	-1.09942000	9.20825000	0.39421900
H	0.34950500	10.04599700	1.75531200
H	-2.32721000	8.11699700	-1.00452100
C	5.74576400	6.89310800	-0.49791900
H	5.07873100	8.37197900	-1.92003600
H	6.08417200	5.34440300	0.96562200
H	-1.79915100	10.03275400	0.49658000
H	6.79970100	7.12479700	-0.62206700
C	-3.73823200	-2.25457200	-0.03987500
C	-4.54933200	-2.77902500	0.98041600
C	-4.38372700	-1.71266300	-1.16429900
C	-5.93837400	-2.73944700	0.89979100
H	-4.08010700	-3.20767400	1.86204700
C	-5.77178300	-1.68377200	-1.26357200
H	-3.78756600	-1.35118600	-1.99850000
C	-6.57444200	-2.19400400	-0.22850700
H	-6.53849900	-3.13521700	1.71264800
H	-6.24124200	-1.28176800	-2.15546200
N	-7.98673400	-2.17028200	-0.32561500
C	-8.75875700	-3.26453500	0.15960800
C	-8.64602200	-1.06755300	-0.93880400
C	-9.93122200	-3.03182500	0.89533700
C	-8.36521900	-4.58730800	-0.09722800
C	-9.68678000	-1.28166500	-1.85590200
C	-8.27088300	0.24929400	-0.62906900
C	-10.69498800	-4.10264500	1.35616100
H	-10.23800100	-2.01091300	1.10002600

C	-9.12566900	-5.65186700	0.38338100
H	-7.46481500	-4.77365800	-0.67407000
C	-10.33872100	-0.19918200	-2.44388400
H	-9.97895800	-2.29761500	-2.10195200
C	-8.91619700	1.32541600	-1.23545100
H	-7.47758700	0.42086800	0.09206000
C	-10.29600700	-5.41778300	1.10843000
H	-11.60042100	-3.90544600	1.92407800
H	-8.80739900	-6.67005500	0.17549300
C	-9.95565000	1.10954000	-2.14283700
H	-11.14254900	-0.38271500	-3.15194300
H	-8.61395300	2.33871100	-0.98384900
H	-10.89000400	-6.24990300	1.47530400
H	-10.46176100	1.95055100	-2.60801900
C	2.04854900	-3.16898100	-0.02081200
C	2.66043600	-4.41299100	-0.08397300
S	3.26521700	-1.90389700	0.02724400
C	4.06644500	-4.36537400	-0.09005800
H	2.10622900	-5.34283800	-0.13011400
C	4.57115100	-3.07668800	-0.03281300
H	4.69290500	-5.25029800	-0.13720800
C	5.94621100	-2.65595900	-0.02336400
C	6.45070900	-1.35859500	0.03334200
S	7.24592800	-3.82755800	-0.08654100
C	7.84980600	-1.30968800	0.02586100
H	5.81530600	-0.48126600	0.07903100
C	8.46711500	-2.55852900	-0.03616400
H	8.42329500	-0.38892500	0.06452400
C	9.87666300	-2.74119600	-0.05423300
C	10.63703400	-3.88282500	-0.11270400
H	10.43880300	-1.81188200	-0.01450000
C	10.07111100	-5.19110600	-0.17024000
C	12.11540600	-3.83378200	-0.11992600
N	9.58413500	-6.24826200	-0.21641000
O	12.84167000	-4.80507100	-0.16981800
O	12.60629800	-2.56342800	-0.06381200
H	13.57543200	-2.66479400	-0.07471700

Dye 7c(total energy= -3494.50176867 a.u)

C	0.69028600	0.81001600	-0.11720400
N	1.54086000	-0.19489100	-0.14380000
N	-0.63538600	0.38985000	-0.19593900
C	0.77833200	-1.33794800	-0.22236400
C	-0.60318900	-1.00177700	-0.27750600
C	1.22673700	-2.68036600	-0.23336100
C	-1.60211700	-1.99845300	-0.38623500
C	0.22029900	-3.65285500	-0.28882400
C	-1.13469400	-3.32285000	-0.36365100

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H	0.49454600	-4.70258400	-0.26016500
H	-1.86547600	-4.12306300	-0.43571100
C	-1.81541300	1.25619900	-0.20524900
C	-2.57337400	1.28867700	1.12839000
H	-2.48465500	0.92133700	-0.99939600
H	-1.47446200	2.25779000	-0.47580800
C	-3.79262800	2.21857800	1.07315100
H	-2.89553200	0.27296300	1.38635100
H	-1.89347200	1.60809800	1.92993400
C	-4.56788600	2.26238700	2.39377700
H	-3.46748200	3.23409000	0.80494000
H	-4.46206900	1.88779500	0.26733100
H	-5.43350900	2.93002900	2.32316200
H	-4.93539600	1.26666700	2.66871600
H	-3.93496600	2.62130500	3.21454100
C	1.14944800	2.20915900	-0.06630700
C	0.55331500	3.21761400	0.70920800
C	2.30702700	2.54386300	-0.79288700
C	1.07413600	4.50683900	0.74145500
H	-0.29918600	2.99188700	1.34107100
C	2.82348800	3.83144200	-0.77843700
H	2.79014500	1.77255300	-1.38334500
C	2.21243500	4.84187800	-0.01201500
H	0.60609500	5.25932100	1.36710800
H	3.70335700	4.06499400	-1.36830600
N	2.73151000	6.15544100	0.00601300
C	1.85529700	7.27483900	0.10596800
C	4.13660700	6.37906500	-0.07813000
C	2.15271300	8.33137700	0.98030100
C	0.69125600	7.34180700	-0.67553800
C	4.64374600	7.38342700	-0.91679300
C	5.02967000	5.60777900	0.68194000
C	1.30279000	9.43288900	1.06467700
H	3.05090400	8.28315700	1.58786700
C	-0.16203100	8.43883400	-0.57134700
H	0.46251100	6.53250800	-1.36183600
C	6.01666800	7.61311200	-0.98589600
H	3.95741100	7.97947400	-1.50992100
C	6.40233800	5.83185200	0.59162800
H	4.64295900	4.83522800	1.33904300
C	0.13916300	9.49200900	0.29499700
H	1.54721600	10.24306900	1.74660400
H	-1.05918100	8.47612500	-1.18371800
C	6.90433200	6.83716800	-0.23763300
H	6.39346600	8.39502000	-1.63997600
H	7.08072400	5.22513000	1.18559000
H	-0.52416900	10.34906000	0.36810000
H	7.97430500	7.01395000	-0.29947600
C	2.65554800	-3.06038500	-0.18747500
C	3.10332700	-4.23395200	-0.82299600

C	3.61465900	-2.29618900	0.50384500
C	4.43362900	-4.63181500	-0.77154300
H	2.40508400	-4.82759900	-1.40603700
C	4.94315100	-2.69813700	0.57635500
H	3.30863200	-1.38075100	0.99457300
C	5.37731700	-3.87214800	-0.06067900
H	4.75136000	-5.52933700	-1.29246800
H	5.65605400	-2.09971000	1.13462600
N	6.73603000	-4.27559700	0.00380600
C	7.06564200	-5.65004300	0.15758100
C	7.77213900	-3.30579700	-0.09322000
C	8.12154800	-6.21724200	-0.57441700
C	6.34181600	-6.46166400	1.04646500
C	8.89616300	-3.37664100	0.74560700
C	7.68783000	-2.26396000	-1.03098100
C	8.44689700	-7.56250000	-0.41195200
H	8.68225400	-5.59814600	-1.26740200
C	6.66312300	-7.81013900	1.18824100
H	5.53014400	-6.02841000	1.62214500
C	9.91412400	-2.43091600	0.63844600
H	8.96505100	-4.17531200	1.47732700
C	8.70229400	-1.31263700	-1.11811500
H	6.82477900	-2.20553900	-1.68635400
C	7.71896700	-8.36934700	0.46516600
H	9.26698700	-7.98432500	-0.98730800
H	6.09200600	-8.42277300	1.88110000
C	9.82361800	-1.39113000	-0.28937100
H	10.77682900	-2.50152900	1.29593800
H	8.61983400	-0.51314400	-1.84987700
H	7.97122600	-9.41925600	0.58384200
H	10.61601400	-0.65190800	-0.36521300
C	-3.04972500	-1.77391800	-0.54718700
C	-3.74111100	-1.14112500	-1.55901400
S	-4.17527300	-2.47448800	0.60066700
C	-5.14987600	-1.20436500	-1.42182800
H	-3.24362400	-0.68725500	-2.40910700
C	-5.56690200	-1.90038100	-0.30279900
H	-5.84027500	-0.77894300	-2.14300300
C	-6.91158600	-2.16673200	0.14581000
C	-7.33098600	-3.04816800	1.13524700
S	-8.27094700	-1.32636300	-0.56402500
C	-8.72250900	-3.05592600	1.31181100
H	-6.64702800	-3.67464800	1.69698500
C	-9.40902400	-2.18512000	0.46939300
H	-9.23729200	-3.68425000	2.03154400
C	-10.82566600	-2.03329500	0.47404200
C	-11.64466300	-1.23360200	-0.27947600
H	-11.33123400	-2.66142600	1.20270600
C	-11.15358600	-0.34429300	-1.28162100
C	-13.11588500	-1.23635900	-0.10256000

N	-10.72374200	0.37288500	-2.09234300
O	-13.88857700	-0.55144200	-0.73900000
O	-13.53124400	-2.09979600	0.86427300
H	-14.50181300	-2.01374500	0.88735200

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