Supporting Information

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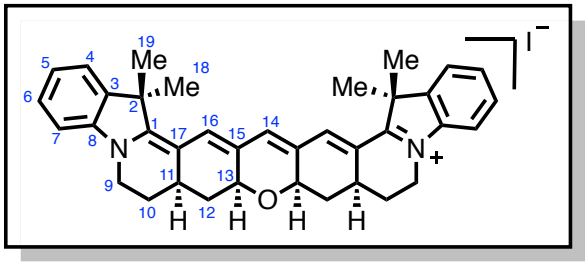
Section S1. NMR Chacterization



Position	δ_H (mult., *J* in Hz)	δ_C (mult., *J* in Hz)
1	–	167.9
2	–	50.0
3	–	143.6 or 142.5
4 – 7	7.47 (d, *J* = 6.9 Hz, 2H), 7.39 (td, *J* = 7.8, 1.2 Hz, 2H), 7.24 (t, *J* = 7.4 Hz, 2H), 7.21 (m, 2H)	143.1, 129.7, 126.1, 123.3
8	–	143.6 or 142.5
9	4.28 (dd, *J* = 13.7, 4.1 Hz, 2H), 3.80 (td, *J* = 13.2, 4.0 Hz, 2H)	44.1
10	2.40 – 2.32 (m, 2H) 1.76 – 1.73 (m, 2H)	28.8
11	2.80 (tt, *J* = 12.4, 4.1 Hz, 2H)	32.6
12	2.44 (dt, *J* = 11.4, 4.3 Hz, 2H) 1.45 (q, *J* = 11.7 Hz, 2H)	36.5
13	–	73.8
14	7.22 (s, 1H)	111.1
15	–	132.7
16	7.50 (s, 2H)	141.3
17	–	115.4
18 – 19	1.70 (d, *J* = 4.5 Hz, 12H)	28.2, 27.7

Figure S1. ^{1}H and ^{13}C NMR assignments of **2** (in MeOD).

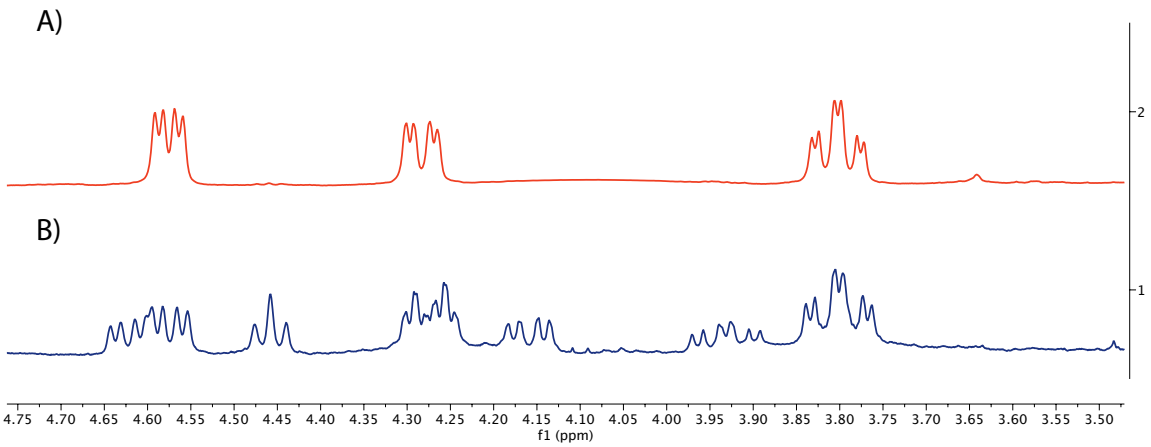
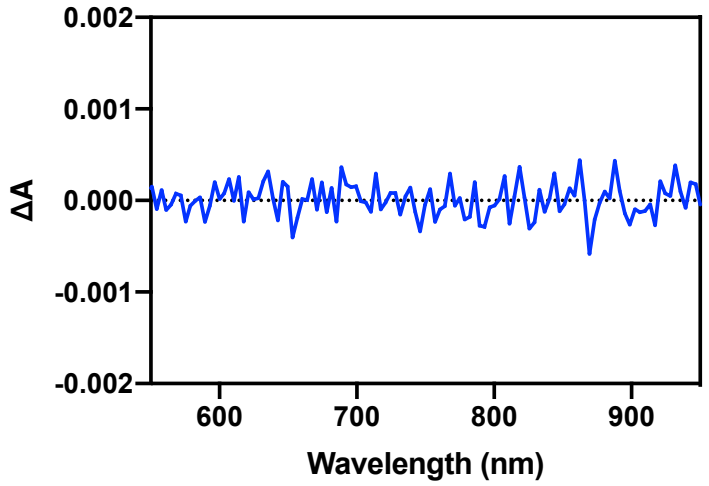


Figure S2. ^{1}H NMR of A) pure equilibrated (red) and B) diastereomeric mixture (blue) of **2** in MeOD.

Section S2. Photophysical measurements

A)



B)

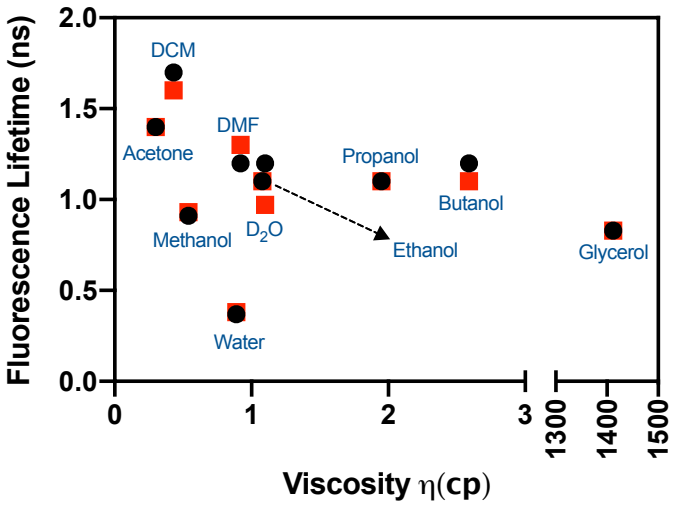


Figure S3. A) Difference transient absorption spectrum of **1** in glycerol at a 50 ns delay time. The positive absorption signal observed with **1** in ethanol (Figure 2A) is not observed in glycerol at any delay time. B) Relationship between Fluorescence lifetime (τ_F) and viscosity for **1** (black circle) and **2** (red square) in different solvents.

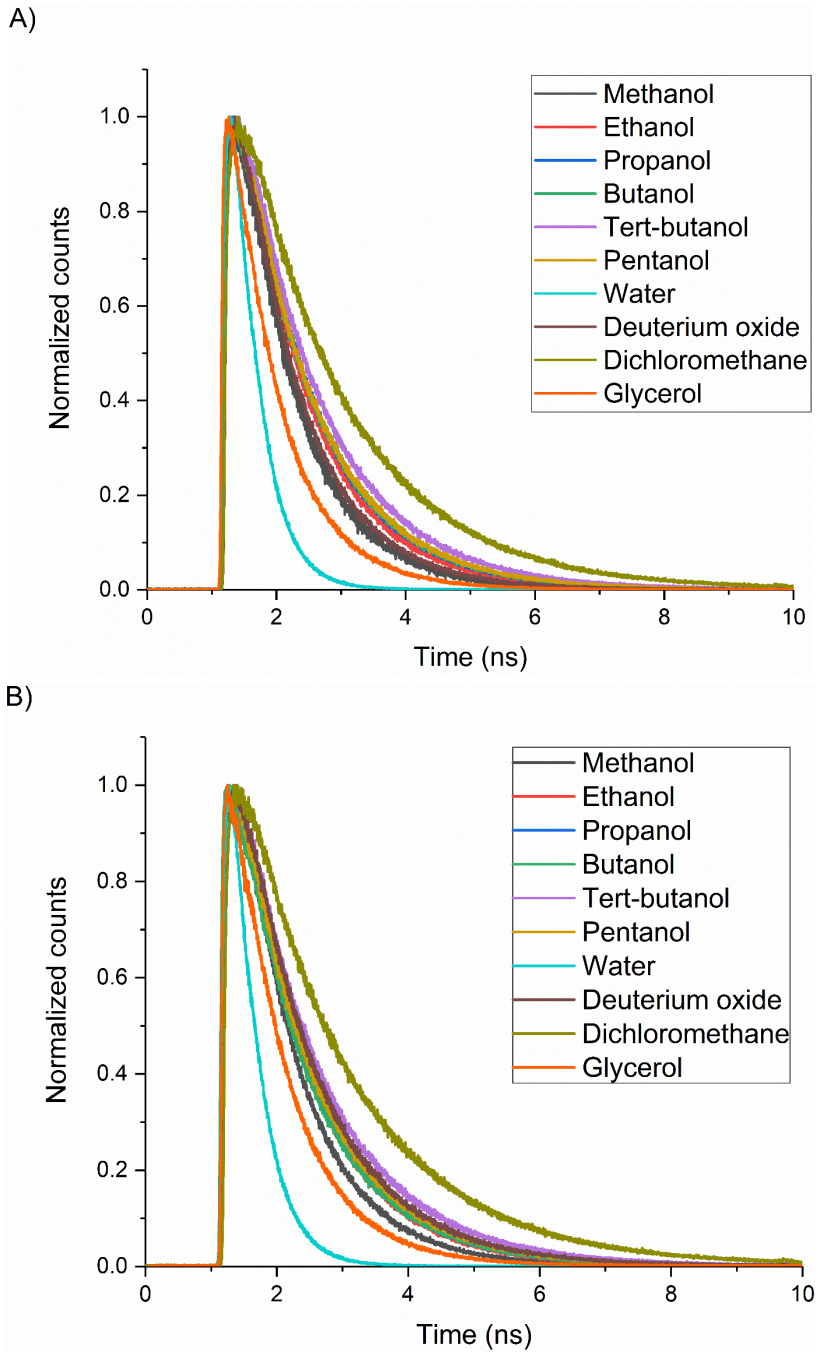


Figure S4. Lifetime data for A) parent heptamethine indocyanine **1** and B) constrained heptamethine indocyanine **2** in different solvent. Lifetimes are listed in Table S1.

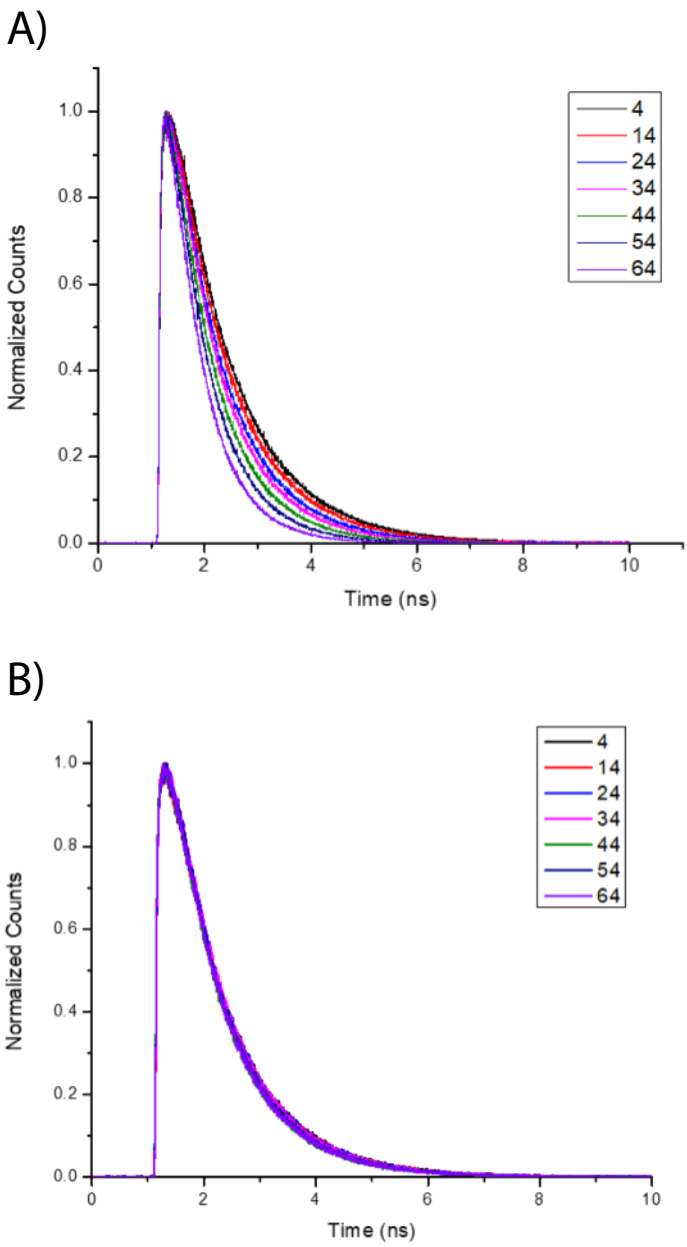


Figure S5. Lifetime data for A) parent heptamethine indocyanine **1** and B) constrained heptamethine indocyanine **2** at different temperatures (as shown in the legend; in ^{o}C) in ethanol.

Table S1. Photophysical data collected for **1** and **2** in protic and aprotic solvents

	Solvents	*Solvent Properties*		*Parent heptamethine indocyanine, 1*			*Conformationally restrained heptamethine indocyanine, 2*		
		Dielectric constant	**Viscosity η(cp)**	**ϕ_F**	**τ_F (ns)**	**ln(k_{nr})**	**ϕ_F**	**τ_F(ns)**	**ln(k_{nr})**
Protic Solvents	Methanol	33.6	0.54	0.24	0.91	-0.180	0.29	0.93	-0.270
	Ethanol	25	1.08	0.24‡	1.1	-0.370	0.31	1.1	-0.466
	Propanol	21.51	1.95	0.26	1.1	-0.396	0.3	1.1	-0.452
	Butanol	18.34	2.59	0.30	1.2	-0.539	0.32	1.1	-0.481
	Tert-butanol	18.74	6.68	0.35	1.2	-0.613	0.34	1.3	-0.678
	Pentanol	15.8	3.5	0.31	1.2	-0.553	0.32	1.2	-0.568
	Water *	80.36	0.89	0.064	0.37	0.928	0.081	0.38	0.883
	Glycerol	42.5	1412	0.26	0.83	-0.115	0.28	0.83	-0.142
Aprotic Solvents	DCM	9.02	0.43	0.46	1.6	-1.086	0.40	1.7	-1.041
	D_2O	78.3	1.1	0.2	0.97	-0.193	0.18	1.2	-0.381
	Acetone	21.36	0.30	0.33	1.4	-0.737	0.37	1.4	-0.799
	DMF	37.06	0.92	0.31	1.3	-0.633	0.34	1.2	-0.598

- *Contains 5% DMSO in all steady-state experiments (no DMSO in lifetime experiments).

Section S3. Computational Chemistry Methods and Results

Quantum chemistry calculations were performed using a local version of the GAMESS package and molecular orbitals were illustrated using MacMolPlt.[1-3] The 6-31G(d) and cc-pVTZ basis sets have been used.[4-5]

Density functional theory (DFT) utilizing the B3LYP functional was used to optimize ground state (S0) geometries.[6-8] The time-dependent density functional theory (TDDFT) method[6-12] was used to compute vertical excitation, or absorbance, energies (S0 → S1*) at ground state (S0) optimized geometries, as well as deexcitation, or emission, energies (S1 → S0*) at singlet excited state optimized geometries (S1).[10-15] Ground state (S0) DFT and excited state (S1) TDDFT computations used the Euler-MacLaurin radial and Lebedev angular grids with respective dimensions (96, 302) and (48, 110).[16-18] All reported DFT and TDDFT results used the cc-pVTZ basis set.

The occupation restricted multiple active space (ORMAS) method with second-order perturbation theory correction (ORMAS-PT2) was also used to compute vertical excitation (absorbance) energies and deexcitation (emission) energies.[19-21] ORMAS-PT2 calculations were performed using the 6-31G(d) basis set at B3LYP/6-31G(d) ground state (S0; vertical excitation energy) and TDDFT-B3LYP/6-31G(d) excited state (S1; deexcitation energy) optimized geometries. For each system the ORMAS active space contained all valence π electrons (*e*), orbitals (*o*) and the associated configuration interaction (CI) spaces were constructed as follows: we start with the (2 electron, 2 orbital) base active space

(HOMO-like orbital + LUMO-like orbital with two electrons, i.e., (2,2) active space)

(doubly occupied valence π orbitals not including HOMO-like orbital)

and apply all single and double excitations out of this reference and into a virtual orbital space containing only the remaining valence π orbitals. HOMO and LUMO refer to the highest occupied molecular orbital and lowest unoccupied molecular orbital, respectively, in a closed-shell wavefunction. These ORMAS wavefunctions represent active spaces of (20*e*, 19*o*), (22*e*, 21*o*), and (24*e*, 23*o*) for the parent and conformationally restrained versions of trimethine, pentamethine, and heptamethine indocyanines, respectively. The ORMAS S0 and S1 wavefunctions were then simultaneously optimized (for orbitals and CI coefficients) by minimizing the average of the energies of the ground (S0) and excited (S1) singlet states. For example, for parent heptamethine indocyanine the $DET/$ORMAS GAMESS input specifications were:

```
$det   ncore=98 nels=24 nact=23 nstate=3 wstate(1)=1,1 $end
$ormas nspace=3 mstart(1)=99,110,112 mine(1)=20,0,0 maxe(1)=22,4,2 $end
```

and for conformationally restrained heptamethine indocyanine they were:

```
$det   ncore=129 nels=24 nact=23 nstate=3 wstate(1)=1,1 $end
$ormas nspace=3 mstart(1)=130,141,143 mine(1)=20,0,0 maxe(1)=22,4,2 $end
```

Subsequent ORMAS-PT2 energies for each state (S0 and S1) were then computed by modeling all single and double valence electron excitations out of the individual S0 and S1 ORMAS reference wavefunctions (1s orbitals were kept core).

All calculations were performed in solvent (water) phases via the polarizable continuum model (PCM) approach for the DFT, TDDFT, ORMAS, and ORMAS-PT2 methods.[22-25] In all cases a high density of tesserae was used (NTSALL = 960 in $TESCAV).

Table S2. Computed absorbance (top section) and emission (bottom section) energies vs. experimentally measured (eV). All calculations included water solvent effects via the Polarizable Continuum Model (PCM). Differences (computed – experimental) given in parentheses and mean unsigned errors (MUEs) shown at bottom of each section.

System/Method		TDDFT-B3LYP-PCM	ORMAS-PT2-PCM	Experiment
Absorbance				
Trimethine indocyanine	Parent	2.631 (0.373)	2.409 (0.151)	2.258[a]
	Conformationally restrained	2.569 (0.347)	2.341 (0.119)	2.222[a]
Pentamethine indocyanine	Parent	2.334 (0.391)	2.088 (0.145)	1.943[b]
	Conformationally restrained	2.240 (0.367)	2.000 (0.127)	1.873[b]
Heptamethine indocyanine	Parent	2.089 (0.404)	1.849 (0.164)	1.685[c]
	Conformationally restrained	1.978 (0.378)	1.749 (0.149)	1.600[c]
MUE		0.377	0.143	
Emission				
Trimethine indocyanine	Parent	2.174 (–0.028)	2.196 (–0.006)	2.202[a]
	Conformationally restrained	2.156 (–0.008)	2.162 (–0.002)	2.164[a]
Pentamethine indocyanine	Parent	1.939 (0.052)	1.969 (0.082)	1.887[b]
	Conformationally restrained	1.884 (0.053)	1.906 (0.075)	1.831[b]
Heptamethine indocyanine	Parent	1.725 (0.117)	1.780 (0.172)	1.608[c]
	Conformationally restrained	1.644 (0.084)	1.693 (0.133)	1.560[c]
MUE		0.057	0.078	

[a] Klehs, K.; Spahn, C.; Endesfelder, U.; Lee, S. F.; Furstenberg, A.; Heilemann, M., Increasing the brightness of cyanine fluorophores for single-molecule and superresolution imaging. *Chemphyschem* **2014,** *15* (4), 637-41.

[b] Michie, M. S.; Gotz, R.; Franke, C.; Bowler, M.; Kumari, N.; Magidson, V.; Levitus, M.; Loncarek, J.; Sauer, M.; Schnermann, M. J., Cyanine Conformational Restraint in the Far-Red Range. *J Am Chem Soc* **2017,** *139* (36), 12406-12409.

[c] This work.

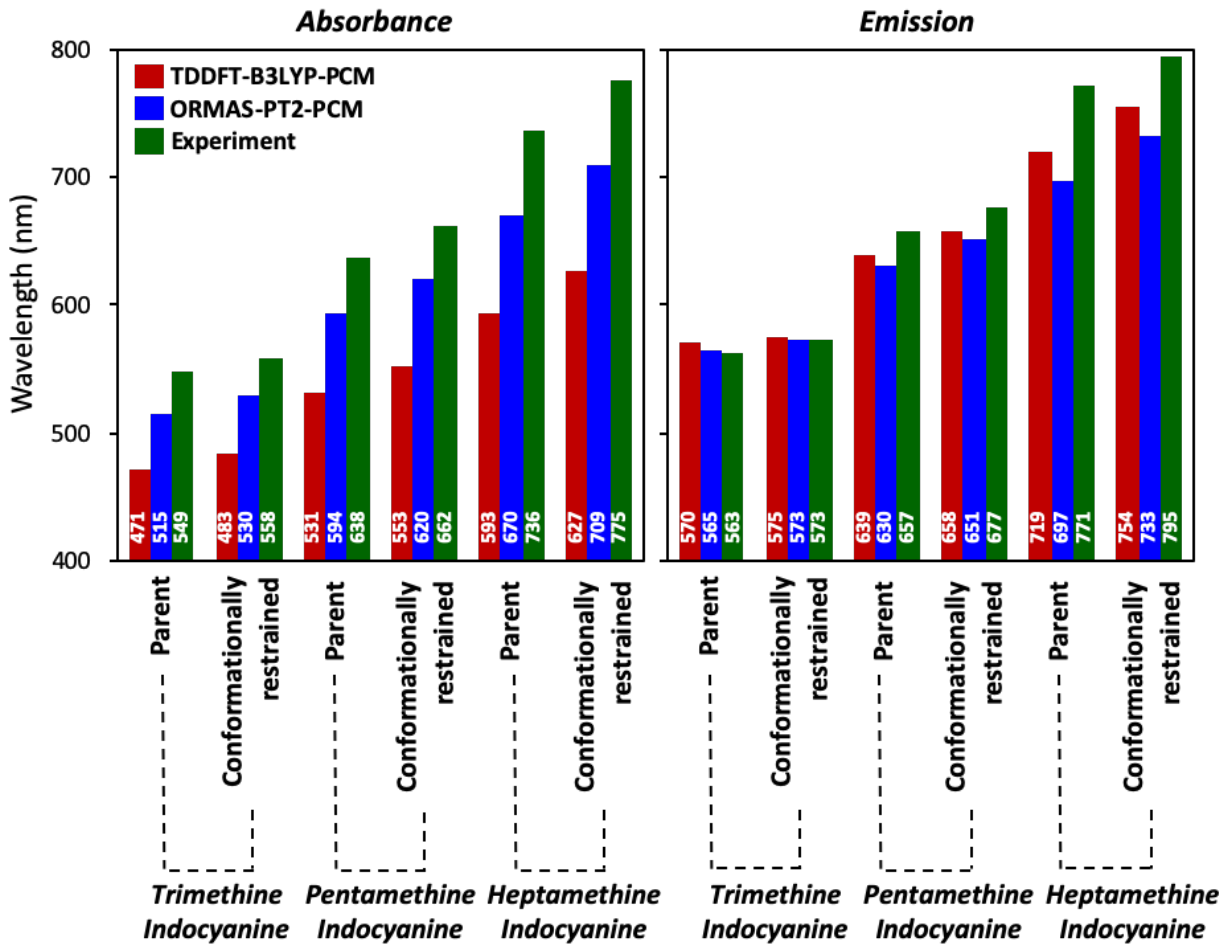


Figure S6 Computed and experimental absorbance and emission energies (nm). See **Table S2** and **Sections S4** and **S5** for more details.

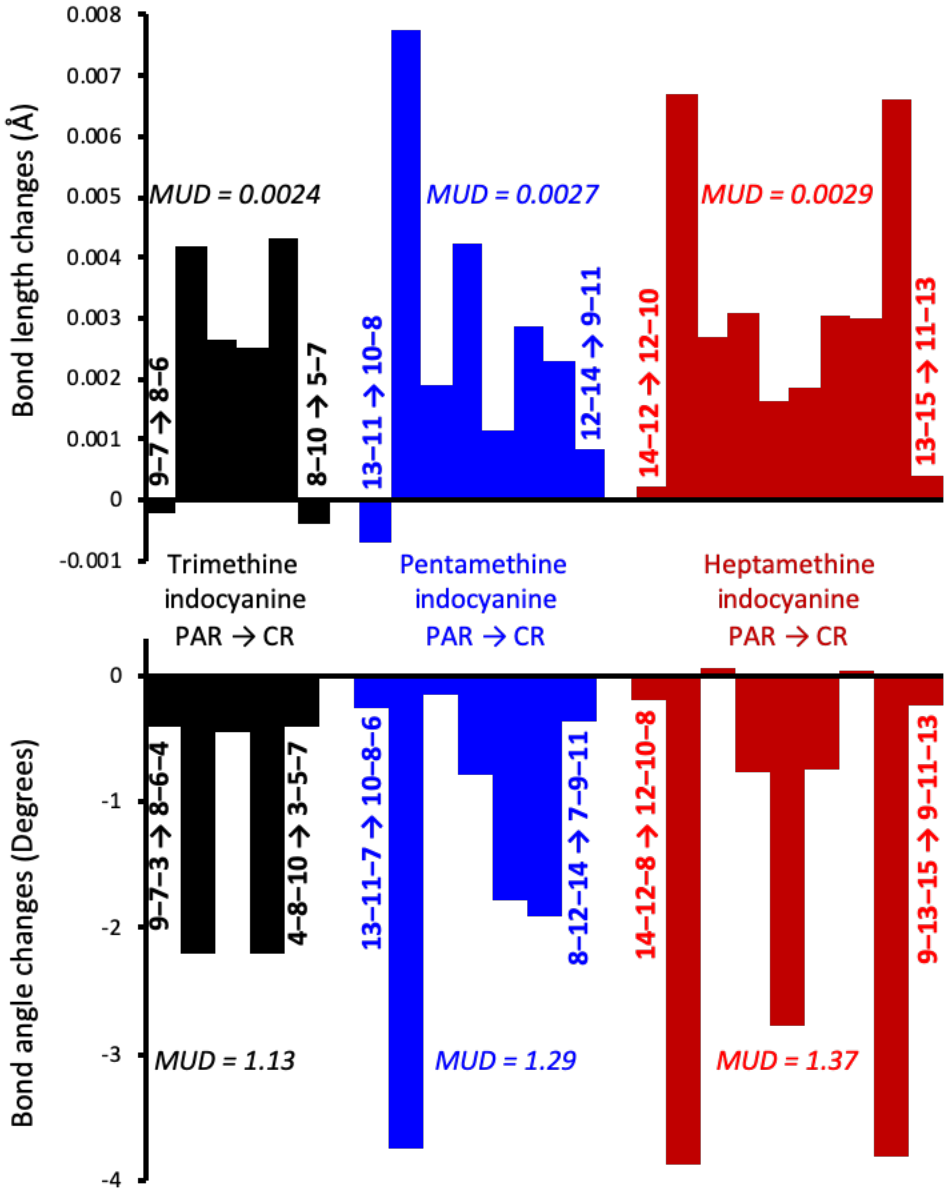
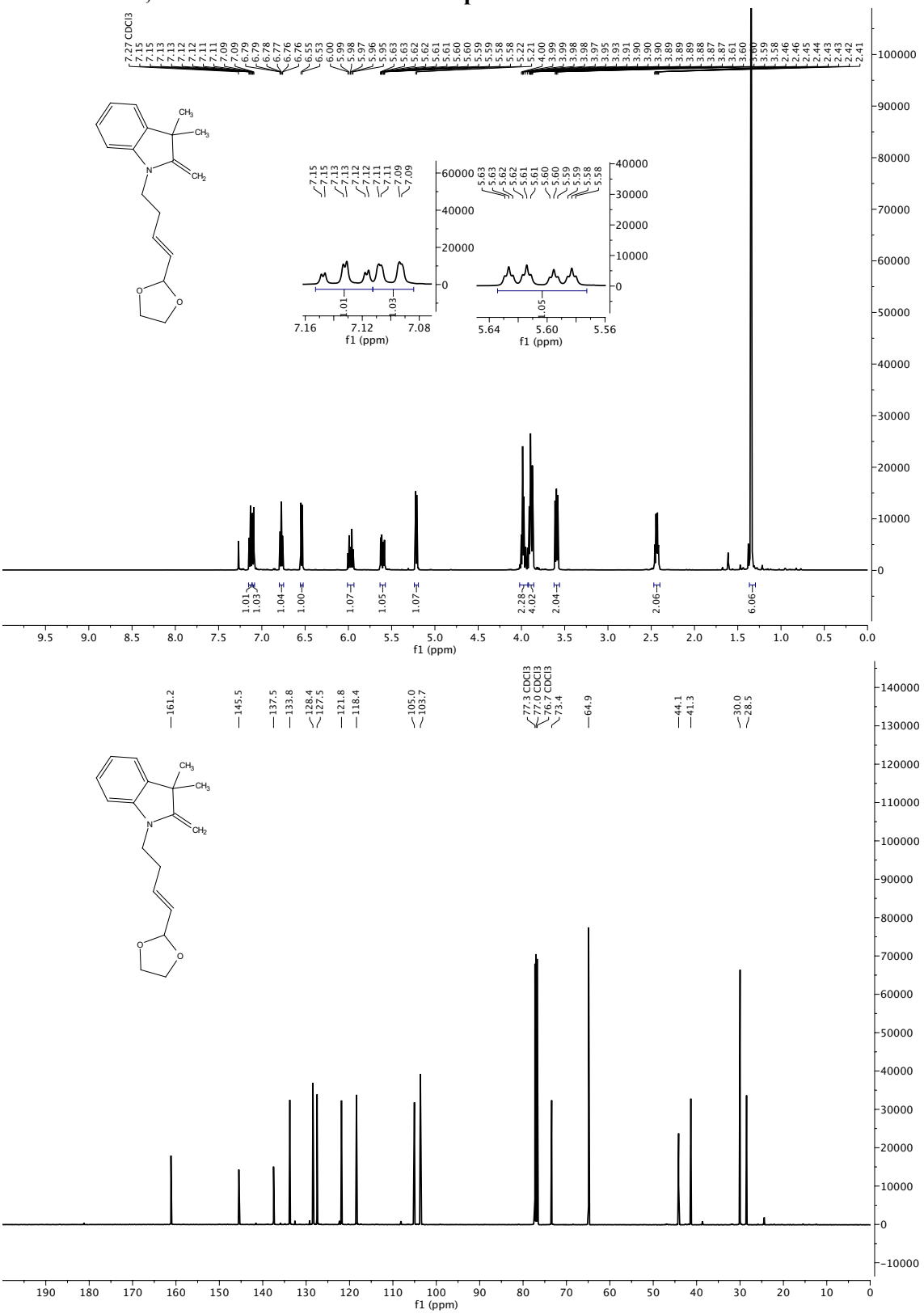
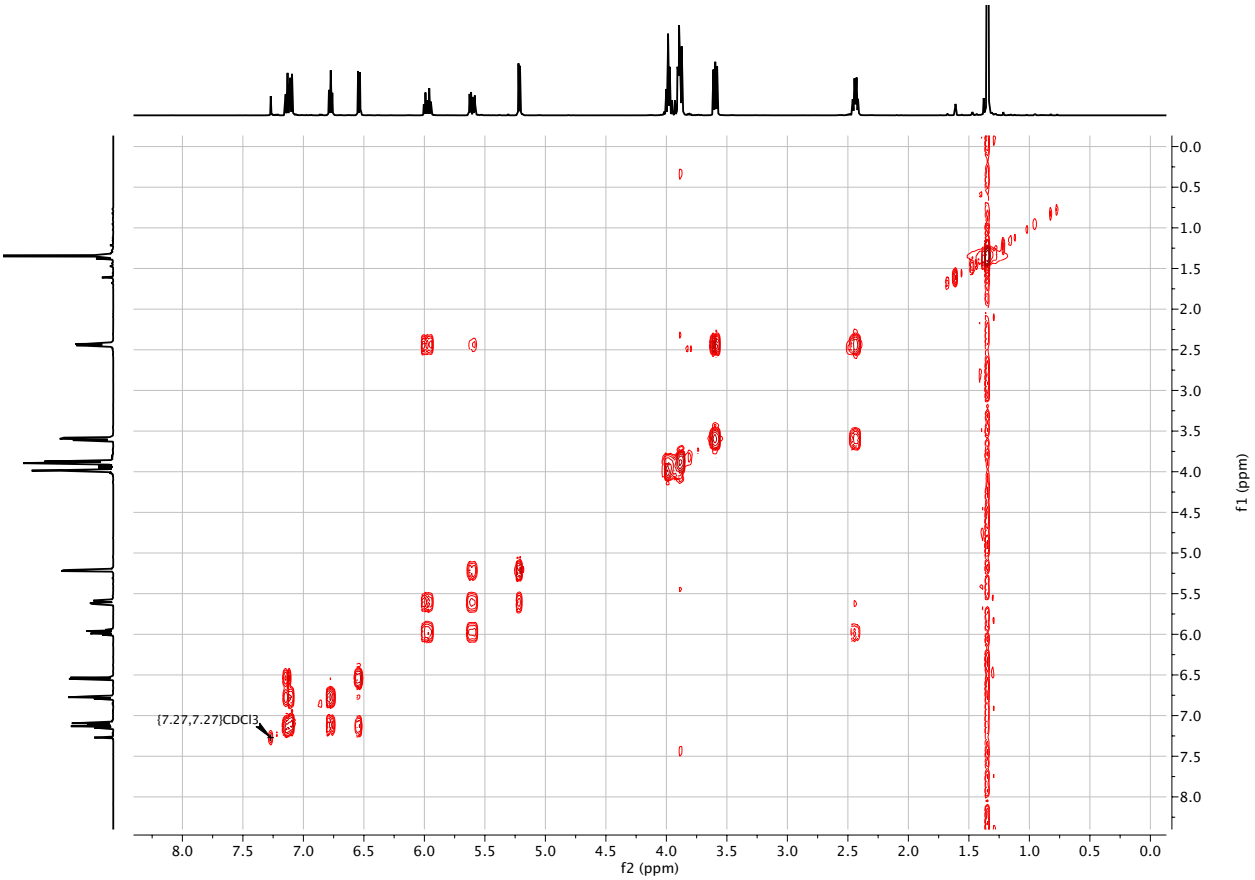


Figure S7. Chain bond length (top) and bond angle (bottom) changes when going from parent indocyanine to its conformationally restricted form. Parameter changes are determined sequentially for heavy atoms starting and ending at nitrogen atoms. Actual start/end bonds and angles are given where atom numberings correspond to the Cartesian coordinates (B3LYP-PCM/cc-pVTZ optimized geometries) provided in **Section S5**. Mean unsigned differences (MUDs) are also shown. **Note: PAR and CR stand for parent and conformationally restrained indocyanine variant.**

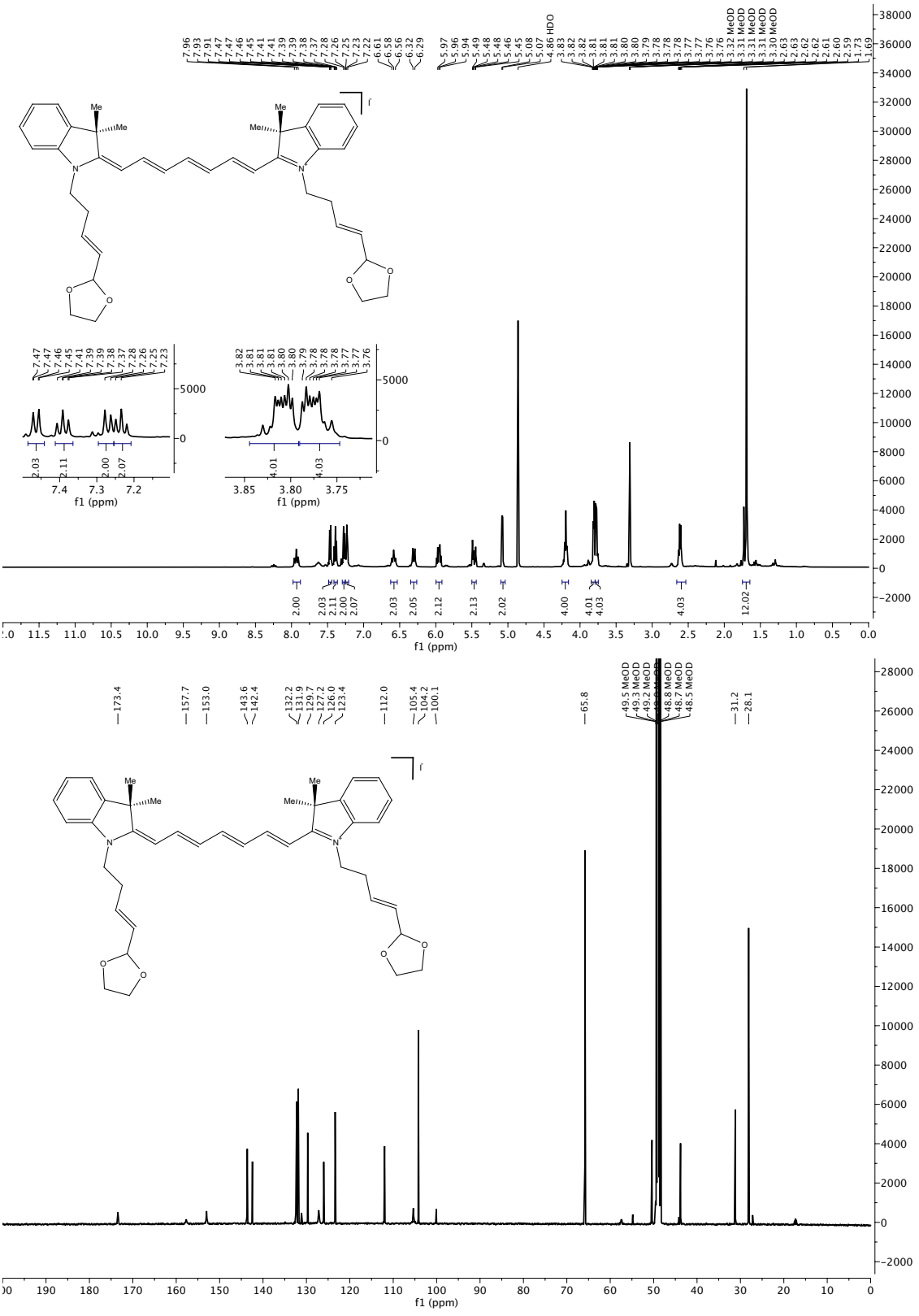
Section S4. ^{1}H, ^{13}C and Associated 2D NMR Spectra



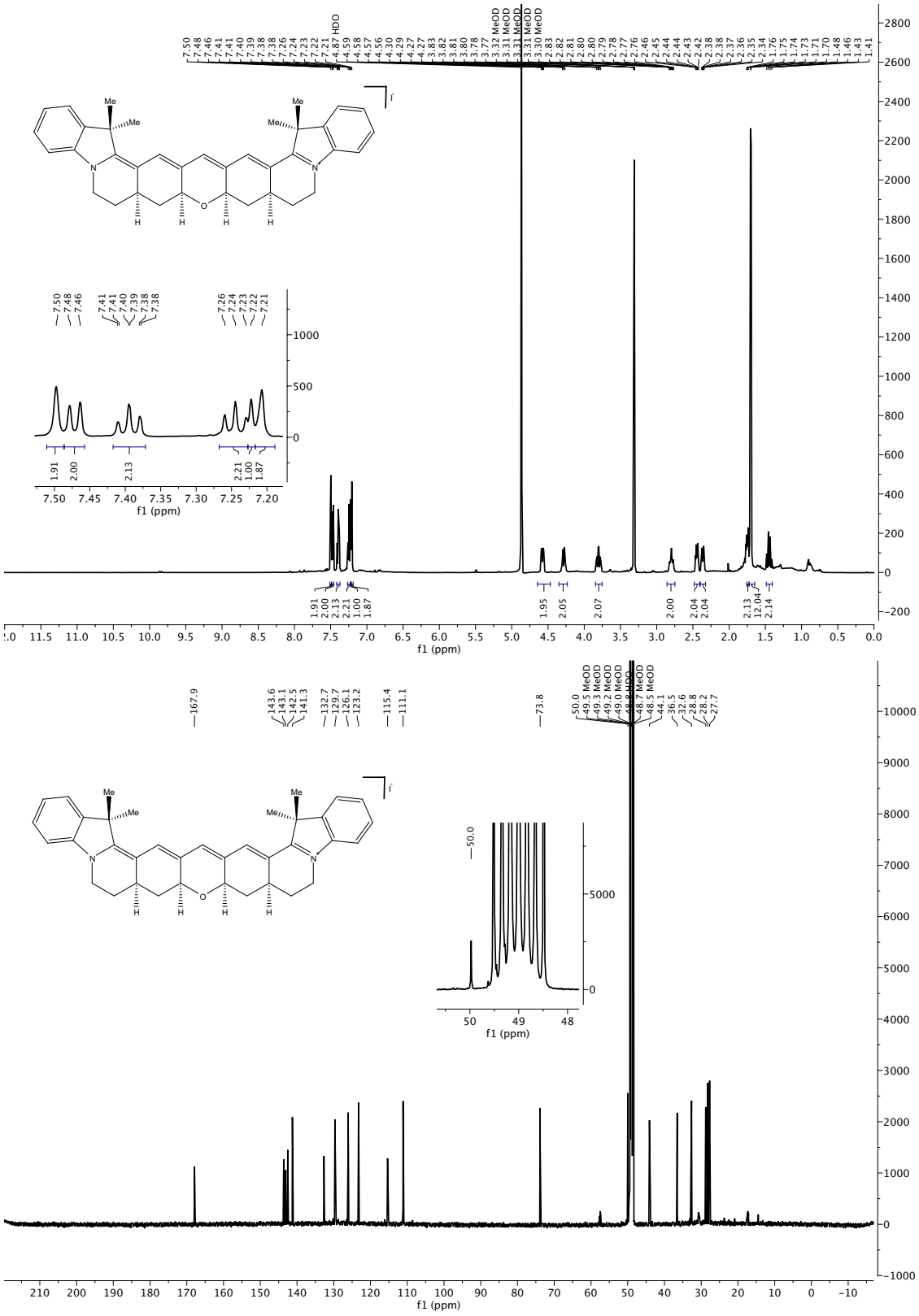
^{1}H (500 MHz) and ^{13}C (126 MHz) NMR spectra of **7**



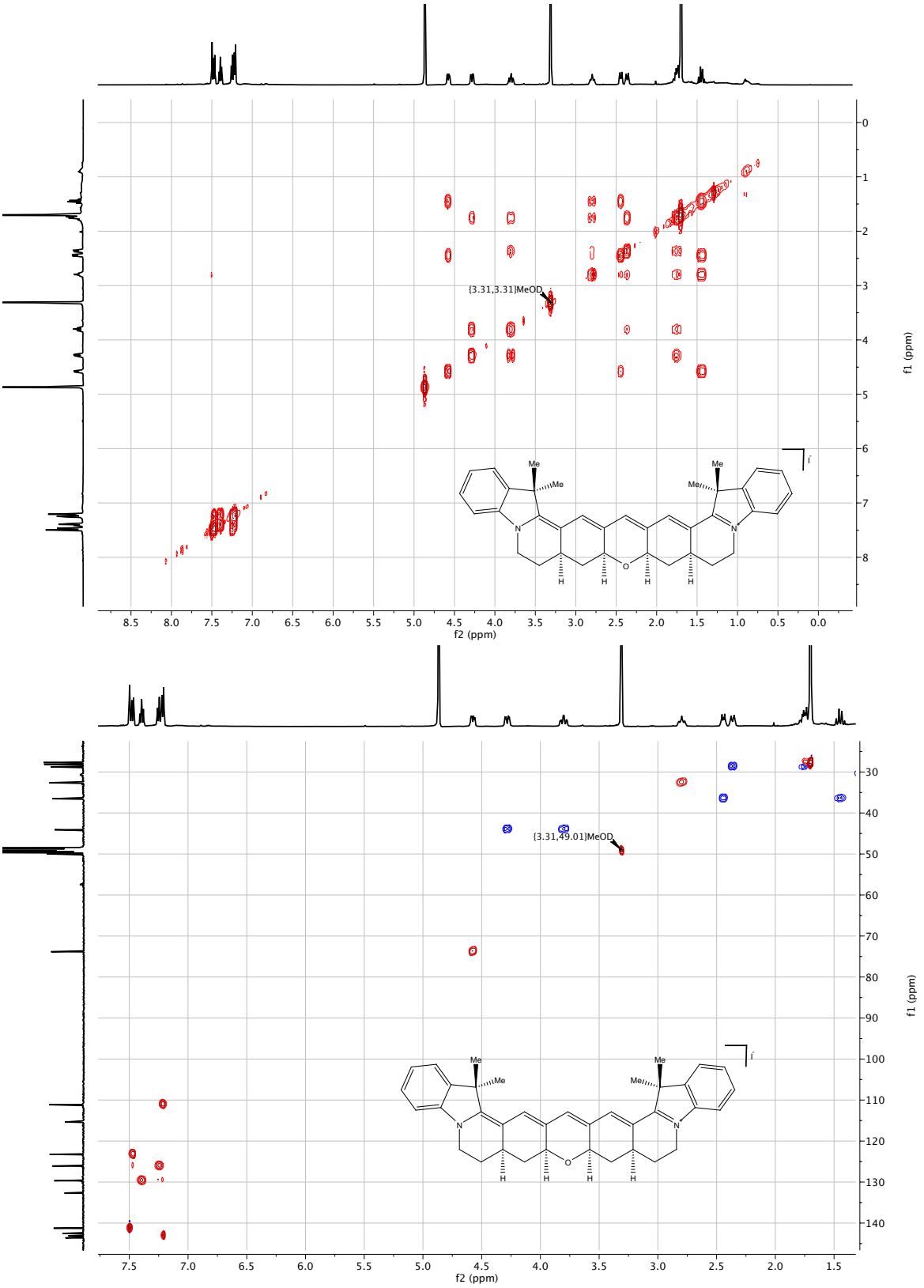
Gradient COSY NMR (500 MHz) spectra of **7**



^{1}H (500 MHz) and ^{13}C (126 MHz) NMR spectra of **3**



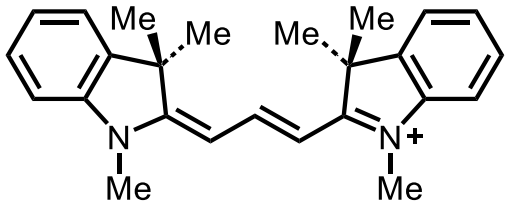
^{1}H (500 MHz) and ^{13}C (126 MHz) NMR spectra of **2**



Gradient COSY (500 MHz) and HSQC (500, 126 MHz) NMR spectra of **2**

Section S5. Raw B3LYP-PCM/cc-pVTZ and TDDFT-B3LYP-PCM/cc-pVTZ Results: Energies (hartree), oscillator strengths, HOMO & LUMO energies (hartree), excitation/de-excitation amplitudes, and optimized structures (Å)

Parent trimethine indocyanine: Results at B3LYP-PCM/cc-pVTZ ground state optimized structure (S0)



E(S0) = -1079.159375
E(S1) = -1079.062671*
Oscillator strength = 1.5256
E(HOMO) = -0.2054; E(LUMO) = -0.1007

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
92	97	0.058653	0.029934
94	97	-0.032767	-0.006865
96	97	0.997968	-0.115547
95	98	0.032897	0.003435
95	100	0.070253	0.015352
96	101	-0.038280	-0.013302

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.0000684525	-0.0014173993	0.5437554308
H	1.0	-0.0001057819	-0.0015830899	-0.5349613092
C	6.0	-1.2213305224	0.0052823679	1.2100361041
C	6.0	1.2212813128	-0.0077583006	1.2099076316
H	1.0	-1.1804789079	0.0039678481	2.2912525550
H	1.0	1.1803386030	-0.0063525535	2.2910967476
C	6.0	-2.4863972383	0.0119927247	0.6302058375
C	6.0	2.4863698660	-0.0134207220	0.6301788138
N	7.0	-3.6064798900	0.0288488932	1.3818235489
N	7.0	3.6064126783	-0.0293606146	1.3819818427
C	6.0	-3.6241552527	0.0512367595	2.8389559919
C	6.0	3.6238203201	-0.0528397607	2.8391130195
H	1.0	-4.6461698971	0.1588289611	3.1822052787
H	1.0	4.6457246583	-0.1606571733	3.1826051780
H	1.0	-3.2117028886	-0.8746861794	3.2393515515
H	1.0	3.0424350852	-0.8965336996	3.2074551754
H	1.0	-3.0427024749	0.8945237672	3.2081965383
H	1.0	3.2112669902	0.8727548114	3.2401538068
C	6.0	-4.7691985431	0.0150380579	0.5844667889

C	6.0	4.7691837665	-0.0135907896	0.5847567756
C	6.0	-6.0988624543	0.0141573643	0.9797806717
C	6.0	6.0988167643	-0.0107169735	0.9802184785
H	1.0	-6.3911753916	0.0213888230	2.0193183536
H	1.0	6.3909348689	-0.0175610476	2.0197988666
C	6.0	-7.0652170506	0.0001372558	-0.0253780537
C	6.0	7.0652943322	0.0047530093	-0.0247985915
H	1.0	-8.1112168133	-0.0012325446	0.2496899191
H	1.0	8.1112620145	0.0076662897	0.2504356785
C	6.0	-6.7057762218	-0.0131518645	-1.3704979250
C	6.0	6.7059847219	0.0175664060	-1.3699510816
H	1.0	-7.4737897300	-0.0240255265	-2.1317924065
H	1.0	7.4740792315	0.0295491399	-2.1311467250
C	6.0	-5.3597420295	-0.0140986547	-1.7436532273
C	6.0	5.3599900364	0.0166400027	-1.7433147855
H	1.0	-5.0871064895	-0.0260079076	-2.7908792333
H	1.0	5.0875569215	0.0281960209	-2.7905967148
C	6.0	-4.3933865962	-0.0008605622	-0.7552764438
C	6.0	4.3935277372	0.0019894802	-0.7550463831
C	6.0	-2.8804268792	-0.0016838576	-0.8530477504
C	6.0	2.8805877873	0.0009670136	-0.8529963413
C	6.0	2.3898215034	1.2815892558	-1.5612844499
C	6.0	-2.3905387055	1.2673112140	-1.5833121630
C	6.0	2.3922066822	-1.2685671650	-1.5833196136
C	6.0	-2.3908824950	-1.2827166686	-1.5614718914
H	1.0	2.7244280875	2.1740425394	-1.0334177025
H	1.0	-2.7267479192	2.1685106731	-1.0715725149
H	1.0	2.7284319746	-2.1693456195	-1.0708244421
H	1.0	-2.7269951414	-2.1749821256	-1.0342551391
H	1.0	2.7911056257	1.3125363323	-2.5739894286
H	1.0	-2.7909581133	1.2800437988	-2.5967846542
H	1.0	2.7936627850	-1.2815152567	-2.5963742181
H	1.0	-2.7915100967	-1.3127663526	-2.5744651749
H	1.0	1.3043296435	1.3139070031	-1.6300157273
H	1.0	-1.3049726083	1.2997605765	-1.6514050571
H	1.0	1.3067201075	-1.3015881361	-1.6525553108
H	1.0	-1.3053799214	-1.3164872337	-1.6293693653

Parent trimethine indocyanine: Results at TDDFT-B3LYP-PCM/cc-pVTZ excited state optimized structure (S1)

E(S0) = -1079.155002*
E(S1) = -1079.075124
Oscillator strength = 1.7383
E(HOMO) = -0.2044; E(LUMO) = -0.1089

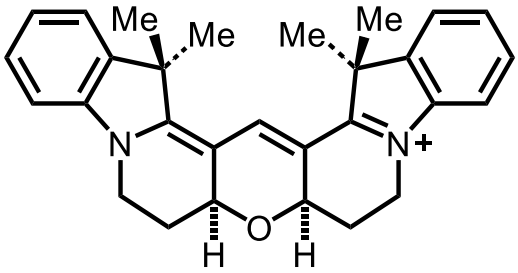
OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
96	97	-0.997532	0.074585
95	98	0.041540	0.006847
95	100	0.058083	0.017526

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.0000170437	-0.0013478253	0.4336801011
H	1.0	-0.0000643937	-0.0019220581	-0.6437512971
C	6.0	-1.2249070556	0.0052594896	1.1213064747
C	6.0	1.2247951050	-0.0070368645	1.1214459491
H	1.0	-1.1570382597	0.0082658542	2.2025410648
H	1.0	1.1565885822	-0.0091983471	2.2026362105
C	6.0	-2.5001225600	0.0082719662	0.5817197163
C	6.0	2.5001540330	-0.0095896890	0.5821451981
N	7.0	-3.6274159241	0.0206264633	1.3867462375
N	7.0	3.6274254773	-0.0208542423	1.3872995450
C	6.0	-3.5881812212	0.0368561568	2.8380991029
C	6.0	3.5880409185	-0.0379800590	2.8386498340
H	1.0	-4.5977873864	0.0788433825	3.2298206856
H	1.0	4.5972879895	-0.0867461301	3.2304547011
H	1.0	-3.1018057162	-0.8639083894	3.2158289751
H	1.0	3.0334457067	-0.9084779108	3.1907685205
H	1.0	-3.0392451369	0.9105518468	3.1913197527
H	1.0	3.1070433047	0.8654173556	3.2171996695
C	6.0	-4.7821611699	0.0136701494	0.6375429993
C	6.0	4.7822183460	-0.0118888709	0.6381466000
C	6.0	-6.1158575063	0.0171499685	1.0647078378
C	6.0	6.1160368584	-0.0128405090	1.0651121643
H	1.0	-6.3805927752	0.0249983317	2.1114674199
H	1.0	6.3811483055	-0.0196599210	2.1117756914
C	6.0	-7.1010375146	0.0083607843	0.0890352396
C	6.0	7.1010440105	-0.0028124150	0.0892180662
H	1.0	-8.1403365091	0.0105636124	0.3883079164
H	1.0	8.1404533050	-0.0030776952	0.3882092989
C	6.0	-6.7776321240	-0.0037507318	-1.2726668436
C	6.0	6.7775579300	0.0082149151	-1.2724883428
H	1.0	-7.5679412956	-0.0103698123	-2.0106677191
H	1.0	7.5677237773	0.0158485062	-2.0106357347

C	6.0	-5.4417179487	-0.0079509368	-1.6847343911
C	6.0	5.4415882063	0.0101866450	-1.6842995010
H	1.0	-5.2014851088	-0.0178561231	-2.7399340597
H	1.0	5.2008652087	0.0194056491	-2.7393653747
C	6.0	-4.4470060149	0.0004164370	-0.7302664172
C	6.0	4.4470688883	0.0006193877	-0.7296616993
C	6.0	-2.9402739720	-0.0022551274	-0.8805264392
C	6.0	2.9404074679	0.0011181328	-0.8799766972
C	6.0	2.4739513197	1.2777325014	-1.6199768820
C	6.0	-2.4729545527	1.2635441913	-1.6388394812
C	6.0	2.4749415780	-1.2657550904	-1.6375857370
C	6.0	-2.4751605163	-1.2795473182	-1.6202757201
H	1.0	2.7999838501	2.1746854837	-1.0944657719
H	1.0	-2.7979617365	2.1683478839	-1.1263491763
H	1.0	2.8012063073	-2.1696564008	-1.1242601866
H	1.0	-2.8019195055	-2.1761935604	-1.0947253517
H	1.0	2.8972700855	1.2948020299	-2.6244713896
H	1.0	-2.8965926116	1.2663724158	-2.6433490598
H	1.0	2.8987726997	-1.2687892818	-2.6420149821
H	1.0	-2.8985256521	-1.2963606025	-2.6247580649
H	1.0	1.3900405646	1.3113199913	-1.7119431795
H	1.0	-1.3889992428	1.2947397452	-1.7315271296
H	1.0	1.3910496557	-1.2985883011	-1.7304016282
H	1.0	-1.3912694289	-1.3140964529	-1.7122799542

Conformationally restrained trimethine indocyanine: Results at B3LYP-PCM/cc-pVTZ ground state optimized structure (S0)



E(S0) = -1307.970228
E(S1) = -1307.875813*
Oscillator strength = 1.4037
E(HOMO) = -0.2019; E(LUMO) = -0.0997

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
109	114	0.050956	0.026607
111	114	-0.032421	-0.007895
113	114	-0.998524	0.119593
112	115	0.036306	0.005004
112	117	0.068714	0.016515
113	118	-0.037710	-0.014603

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0008106668	-0.0107380756	0.6218213552
H	1.0	0.0007276623	-0.0674928641	-0.4532265962
C	6.0	-1.2201248229	0.0128087081	1.2935819257
C	6.0	1.2219682783	0.0161125419	1.2933062996
C	6.0	-2.4682380464	-0.0200456565	0.6693411824
C	6.0	2.4698710635	-0.0178243013	0.6689033331
N	7.0	-3.6075307948	-0.0464328953	1.3906239478
N	7.0	3.6095468774	-0.0367477412	1.3900306869
C	6.0	-4.7499797362	-0.0159648364	0.5728235563
C	6.0	4.7516786874	-0.0124645238	0.5716761834
C	6.0	-6.0837850454	-0.0047012320	0.9520992187
C	6.0	6.0856724412	0.0022569238	0.9502428916
H	1.0	-6.3848297712	-0.0125191722	1.9894730216
H	1.0	6.3870655751	0.0034258354	1.9875282239
C	6.0	-7.0339524192	0.0235990090	-0.0682778992
C	6.0	7.0355050704	0.0214547873	-0.0706302480
H	1.0	-8.0845235054	0.0340742275	0.1886841709
H	1.0	8.0861416863	0.0339928294	0.1860142387
C	6.0	-6.6512174291	0.0407183364	-1.4070294565
C	6.0	6.6523055265	0.0269273338	-1.4093255612

H	1.0	-7.4070118062	0.0628522927	-2.1802340023
H	1.0	7.4078132686	0.0421940501	-2.1829761338
C	6.0	-5.2991057932	0.0323760670	-1.7614113505
C	6.0	5.3000398440	0.0156108322	-1.7631318076
H	1.0	-5.0123282200	0.0478082976	-2.8047522366
H	1.0	5.0130535420	0.0218682496	-2.8065211023
C	6.0	-4.3481027145	0.0065869101	-0.7585269230
C	6.0	4.3493558768	-0.0016478261	-0.7597295891
C	6.0	-2.8313599081	-0.0057370136	-0.8255837006
C	6.0	2.8325861997	-0.0145099514	-0.8262354216
C	6.0	2.3201822154	1.2552150785	-1.5372647440
C	6.0	-2.3184563718	1.2684363349	-1.5279765314
C	6.0	2.3448705493	-1.2958404179	-1.5365210805
C	6.0	-2.3444127067	-1.2824710322	-1.5449152718
H	1.0	2.6558937673	2.1550646722	-1.0228722765
H	1.0	-2.6548984118	2.1649995870	-1.0083649693
H	1.0	2.6917932309	-2.1881981841	-1.0165360378
H	1.0	-2.6923543106	-2.1782727227	-1.0315974842
H	1.0	2.7055348084	1.2802457785	-2.5563326682
H	1.0	-2.7025933803	1.2997077704	-2.5473234226
H	1.0	2.7377931294	-1.3180771366	-2.5527865730
H	1.0	-2.7370039345	-1.2969884764	-2.5614530416
H	1.0	1.2337225274	1.2790182710	-1.5895801859
H	1.0	-1.2319349731	1.2927556193	-1.5786905166
H	1.0	1.2593233533	-1.3374885243	-1.5967618444
H	1.0	-1.2589020571	-1.3248329386	-1.6050904688
C	6.0	3.6667448204	-0.0705022893	2.8527279692
C	6.0	1.1820896095	0.0650596457	2.8127100954
C	6.0	-1.1817908599	0.0561375925	2.8131930081
C	6.0	-3.6656620289	-0.0982231425	2.8527373019
C	6.0	-2.3734581738	-0.6695359988	3.4124565648
C	6.0	2.3791070500	-0.6471382542	3.4172650744
O	8.0	0.0024557705	-0.5624607965	3.3022922402
H	1.0	4.5181509830	-0.6827899132	3.1422004103
H	1.0	3.8443285070	0.9433458951	3.2187943635
H	1.0	2.3121619718	-1.7118999736	3.1875449988
H	1.0	2.3774133893	-0.5342114144	4.5002940675
H	1.0	1.1817126691	1.1137170703	3.1424362221
H	1.0	-4.5116233364	-0.7221322504	3.1335034564
H	1.0	-3.8538375105	0.9091059810	3.2310794915
H	1.0	-2.2985221071	-1.7319317359	3.1745165924
H	1.0	-2.3725289985	-0.5649234554	4.4963229334
H	1.0	-1.1919470643	1.1035072682	3.1470932198

Conformationally restrained trimethine indocyanine: Results at TDDFT-B3LYP-PCM/cc-pVTZ excited state optimized structure (S1)

E(S0) = -1307.966380
E(S1) = -1307.887155*
Oscillator strength = 1.6829
E(HOMO) = -0.2016; E(LUMO) = -0.1074

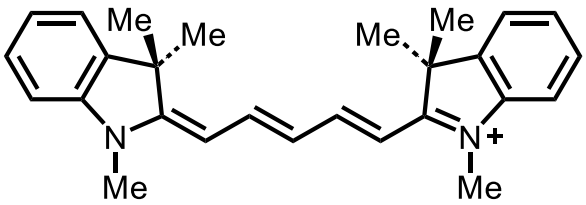
OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
109	114	0.030230	0.024942
113	114	0.997402	-0.080329
112	115	0.048019	0.009636
112	117	0.056938	0.018323
113	118	0.032026	0.013626

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0006325837	-0.0474689805	0.5735377051
H	1.0	0.0005268395	-0.1047959473	-0.5004031812
C	6.0	-1.2306472016	-0.0180618836	1.2547626690
C	6.0	1.2319212892	-0.0217372085	1.2543797645
C	6.0	-2.4836062289	-0.0292438090	0.6465482498
C	6.0	2.4849050614	-0.0320391010	0.6458104997
N	7.0	-3.6410660369	-0.0400015807	1.4012567361
N	7.0	3.6423495614	-0.0502444537	1.4002399437
C	6.0	-4.7664440698	-0.0064480344	0.6136592775
C	6.0	4.7676148213	-0.0099105440	0.6127293757
C	6.0	-6.1097595265	0.0178000515	1.0041991664
C	6.0	6.1109041407	0.0115535979	1.0034403619
H	1.0	-6.3997558860	0.0218479447	2.0445892021
H	1.0	6.4006282537	0.0068295663	2.0438839241
C	6.0	-7.0639070912	0.0436084262	-0.0026820740
C	6.0	7.0651006961	0.0464008094	-0.0031291489
H	1.0	-8.1123654906	0.0632821160	0.2623506693
H	1.0	8.1135187564	0.0645010535	0.2622345787
C	6.0	-6.6960412910	0.0480584207	-1.3525151381
C	6.0	6.6971859169	0.0619794069	-1.3528323672
H	1.0	-7.4623968216	0.0690776567	-2.1151449236
H	1.0	7.4635399082	0.0898297741	-2.1152547655
C	6.0	-5.3473968670	0.0286221013	-1.7245766463
C	6.0	5.3485311840	0.0450608705	-1.7251131014
H	1.0	-5.0759564257	0.0346990384	-2.7721131611
H	1.0	5.0772274296	0.0597800201	-2.7725982499
C	6.0	-4.3829212420	0.0037361687	-0.7393057162
C	6.0	4.3840459278	0.0117529233	-0.7400339958
C	6.0	-2.8694938759	-0.0214891436	-0.8341980391
C	6.0	2.8706009452	-0.0128966387	-0.8348673060

C	6.0	2.3586513087	1.2557694337	-1.5571105533
C	6.0	-2.3579234484	1.2416440572	-1.5665300324
C	6.0	2.4059523158	-1.2886648701	-1.5791682678
C	6.0	-2.4045140088	-1.3027826446	-1.5686229087
H	1.0	2.6841275454	2.1577182333	-1.0399933650
H	1.0	-2.6826461458	2.1476468903	-1.0561043107
H	1.0	2.7556111082	-2.1864231733	-1.0705635108
H	1.0	-2.7555752765	-2.1966894201	-1.0542613412
H	1.0	2.7522869583	1.2814004121	-2.5733707861
H	1.0	-2.7524704256	1.2596064903	-2.5826070482
H	1.0	2.8098655959	-1.2883174588	-2.5917939093
H	1.0	-2.8067154012	-1.3093928573	-2.5819106098
H	1.0	1.2723254189	1.2709299621	-1.6175712857
H	1.0	-1.2716589293	1.2561370730	-1.6281798020
H	1.0	1.3212878820	-1.3379292486	-1.6512645142
H	1.0	-1.3197693619	-1.3532695931	-1.6383867990
C	6.0	3.6630506551	-0.0728201563	2.8597027206
C	6.0	1.1802685629	0.0189000881	2.7717193909
C	6.0	-1.1770819635	0.0274470305	2.7719420218
C	6.0	-3.6602933138	-0.0469417939	2.8608448825
C	6.0	-2.3773469079	-0.6600496476	3.3982139827
C	6.0	2.3760575875	-0.6810906338	3.3928995618
O	8.0	-0.0005113631	-0.6074823054	3.2539885688
H	1.0	4.5264295826	-0.6509516351	3.1825766908
H	1.0	3.7904423294	0.9503273502	3.2267260669
H	1.0	2.3326713472	-1.7451961290	3.1547255342
H	1.0	2.3492102289	-0.5749253601	4.4763364986
H	1.0	1.1731924112	1.0719311533	3.0939286725
H	1.0	-4.5279416409	-0.6143337275	3.1909756357
H	1.0	-3.7785401358	0.9812830231	3.2166575476
H	1.0	-2.3412657118	-1.7260779733	3.1674529885
H	1.0	-2.3495014578	-0.5465702524	4.4808953665
H	1.0	-1.1597462260	1.0813241116	3.0906577044

Parent pentamethine indocyanine: Results at B3LYP-PCM/cc-pVTZ ground state optimized structure (S0)



E(S0) = -1156.545039
E(S1) = -1156.459258*
Oscillator strength = 2.1258
E(HOMO) = -0.1964; E(LUMO) = -0.1061

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
99	104	-0.048927	-0.024463
101	104	0.048157	0.017417
103	104	-0.999937	0.138223
102	105	0.087839	0.018601
102	107	-0.038183	-0.011681
103	108	-0.038352	-0.014346

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000245496	0.0000083120	-1.2096624519
H	1.0	-0.0000517985	0.0000115479	-2.2951531647
C	6.0	-1.2202450956	0.0000129316	-0.5448297365
C	6.0	1.2204355744	-0.0000022047	-0.5450248146
H	1.0	-1.1849291834	0.0000054919	0.5371220212
H	1.0	1.1852155450	-0.0000020078	0.5369284165
C	6.0	-2.4545203942	0.0000264034	-1.1904551055
C	6.0	2.4546020662	-0.0000150938	-1.1907969676
H	1.0	-2.4322133959	0.0000401862	-2.2724608572
H	1.0	2.4321813569	-0.0000204268	-2.2727823145
C	6.0	-3.7063200401	0.0000214604	-0.5876388194
C	6.0	3.7064541692	-0.0000203280	-0.5880230468
N	7.0	-4.8436725143	0.0000469901	-1.3174774736
N	7.0	4.8438231019	-0.0000535342	-1.3177779701
C	6.0	-4.8891118005	0.0000921963	-2.7732671058
C	6.0	4.8892329215	-0.0000998045	-2.7735899960
H	1.0	-5.9224973844	0.0001582263	-3.0985643557
H	1.0	5.9226286177	-0.0002577432	-3.0988718367
H	1.0	-4.3976651205	0.8887720901	-3.1683552065
H	1.0	4.3979871826	0.8886662848	-3.1687217779
H	1.0	-4.3977573076	-0.8886146241	-3.1684105475
H	1.0	4.3977455751	-0.8887552693	-3.1686660814

C	6.0	-5.9879839136	0.0000172870	-0.4964414538
C	6.0	5.9881544328	-0.0000214589	-0.4966696576
C	6.0	-7.3256600829	0.0000213600	-0.8648961350
C	6.0	7.3259183663	-0.0000243447	-0.8648727823
H	1.0	-7.6383805559	0.0000500803	-1.8985154778
H	1.0	7.6391079747	-0.0000505239	-1.8983461023
C	6.0	-8.2721043473	-0.0000160222	0.1589208984
C	6.0	8.2721204364	0.0000125893	0.1591922871
H	1.0	-9.3233298526	-0.0000148613	-0.0959410948
H	1.0	9.3234139959	0.0000121382	-0.0953599182
C	6.0	-7.8862246269	-0.0000558151	1.4965882562
C	6.0	7.8860126213	0.0000517387	1.4968028737
H	1.0	-8.6391293594	-0.0000851463	2.2729363364
H	1.0	8.6387823485	0.0000808499	2.2732888802
C	6.0	-6.5325261334	-0.0000590065	1.8429994249
C	6.0	6.5322721388	0.0000557405	1.8429258408
H	1.0	-6.2397254067	-0.0000909025	2.8848704000
H	1.0	6.2390951064	0.0000883519	2.8846829953
C	6.0	-5.5850322700	-0.0000227192	0.8362415527
C	6.0	5.5850186006	0.0000199594	0.8359654840
C	6.0	-4.0700616359	-0.0000184931	0.9035365627
C	6.0	4.0700634022	0.0000186045	0.9031591606
C	6.0	-3.5624196838	1.2738878446	1.6133140531
C	6.0	3.5623028231	1.2738782945	1.6129493120
C	6.0	-3.5624086434	-1.2739543810	1.6132510284
C	6.0	3.5623086686	-1.2738096449	1.6130123006
H	1.0	-3.9061364683	2.1714781886	1.0998315269
H	1.0	3.9061673076	2.1715648723	1.0997555664
H	1.0	-3.9061195296	-2.1715221903	1.0997251934
H	1.0	3.9061773959	-2.1715194064	1.0998620906
H	1.0	-3.9453395357	1.2969665869	2.6335866525
H	1.0	3.9449349171	1.2967431297	2.6333356391
H	1.0	-3.9453262303	-1.2970855969	2.6335232794
H	1.0	3.9449415880	-1.2966231518	2.6333994564
H	1.0	-2.4755458116	1.3009918686	1.6603202063
H	1.0	2.4754220013	1.3010046076	1.6596558826
H	1.0	-2.4755345838	-1.3010522548	1.6602535894
H	1.0	2.4754279188	-1.3009392556	1.6597212133

Parent pentamethine indocyanine: Results at TDDFT-B3LYP-PCM/cc-pVTZ excited state optimized structure (S1)

E(S0) = -1156.542603*
E(S1) = -1156.471347
Oscillator strength = 2.3036
E(HOMO) = -0.1967; E(LUMO) = -0.1116

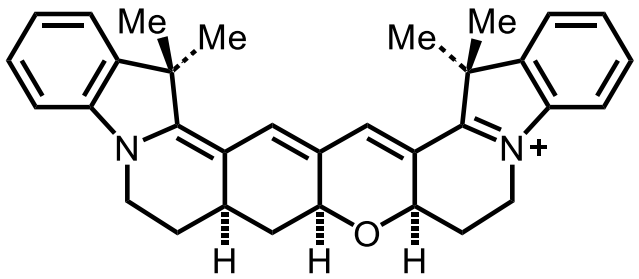
OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
103	104	0.997242	-0.080006
102	105	-0.078320	-0.020535
102	107	0.033798	0.013259

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000100271	0.0030620965	-1.0647850585
H	1.0	-0.0000698699	0.0021633058	-2.1514067258
C	6.0	-1.2327877523	0.0060244410	-0.4121935400
C	6.0	1.2328684171	0.0007153374	-0.4123763129
H	1.0	-1.2198644278	0.0058486540	0.6692997070
H	1.0	1.2200042248	0.0025881409	0.6691135663
C	6.0	-2.4586246279	0.0095911938	-1.0960330549
C	6.0	2.4586836957	-0.0051543783	-1.0962797962
H	1.0	-2.3983158649	0.0125174244	-2.1776024940
H	1.0	2.3985098875	-0.0091531508	-2.1778778444
C	6.0	-3.7287545812	0.0089553125	-0.5432235259
C	6.0	3.7287534995	-0.0063618376	-0.5433664243
N	7.0	-4.8592046805	0.0188164890	-1.3283517198
N	7.0	4.8591947568	-0.0186577973	-1.3283943471
C	6.0	-4.8416820808	0.0380974439	-2.7810785009
C	6.0	4.8417567092	-0.0362770027	-2.7811363362
H	1.0	-5.8568457826	0.0928084277	-3.1563214207
H	1.0	5.8571876852	-0.0870797475	-3.1562729631
H	1.0	-4.2889868325	0.9067392730	-3.1399431749
H	1.0	4.3686849622	0.8678323763	-3.1671936034
H	1.0	-4.3713494633	-0.8669711818	-3.1683730741
H	1.0	4.2921348408	-0.9063030138	-3.1414822208
C	6.0	-6.0111820500	0.0051963044	-0.5616253935
C	6.0	6.0112017572	-0.0086493655	-0.5616365516
C	6.0	-7.3464157810	0.0026313446	-0.9732406544
C	6.0	7.3463848296	-0.0103399582	-0.9732997265
H	1.0	-7.6239072381	0.0098428673	-2.0167508467
H	1.0	7.6237755676	-0.0188881519	-2.0168408657
C	6.0	-8.3219025759	-0.0116939633	0.0152160841
C	6.0	8.3219581690	0.0014705634	0.0150807543
H	1.0	-9.3645105112	-0.0142541709	-0.2726587011
H	1.0	9.3645172654	0.0007505938	-0.2728877222

C	6.0	-7.9824734480	-0.0235311272	1.3706923578
C	6.0	7.9825583646	0.0148027529	1.3705418681
H	1.0	-8.7631502274	-0.0345542002	2.1189159834
H	1.0	8.7632637520	0.0238126801	2.1187540995
C	6.0	-6.6414440512	-0.0220489048	1.7655306807
C	6.0	6.6415416089	0.0172987014	1.7654207339
H	1.0	-6.3869856592	-0.0320906862	2.8173915114
H	1.0	6.3873180631	0.0283761250	2.8173486178
C	6.0	-5.6586348019	-0.0082433111	0.7974568610
C	6.0	5.6586394814	0.0059878896	0.7974208300
C	6.0	-4.1494779296	-0.0048751947	0.9264645717
C	6.0	4.1494436887	0.0068864635	0.9264025077
C	6.0	-3.6746936176	1.2623580231	1.6764294988
C	6.0	3.6706084943	1.2848746949	1.6548307592
C	6.0	-3.6674204557	-1.2812742586	1.6554589265
C	6.0	3.6711637719	-1.2585083669	1.6772808584
H	1.0	-4.0077521208	2.1657602658	1.1663133223
H	1.0	4.0017314604	2.1806776545	1.1303024046
H	1.0	-3.9964250851	-2.1780402783	1.1312127743
H	1.0	4.0022082141	-2.1632984753	1.1683596973
H	1.0	-4.0887188749	1.2660956161	2.6850317878
H	1.0	4.0834997857	1.3063267016	2.6636588770
H	1.0	-4.0802895945	-1.3033093730	2.6642819270
H	1.0	4.0846433493	-1.2621653805	2.6861036532
H	1.0	-2.5897797174	1.2940495408	1.7569506985
H	1.0	2.5855687963	1.3150255517	1.7337557518
H	1.0	-2.5823127219	-1.3087983866	1.7344304704
H	1.0	2.5861472995	-1.2874625843	1.7572665871

Conformationally restrained pentamethine indocyanine: Results at B3LYP-PCM/cc-pVTZ ground state optimized structure (S0)



E(S0) = -1462.755843
E(S1) = -1462.673517*
Oscillator strength = 1.9241
E(HOMO) = -0.1904; E(LUMO) = -0.1041

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
125	128	0.055652	0.023427
127	128	1.001764	-0.146502
126	129	-0.085669	-0.020410
126	131	0.034886	0.011678
127	132	0.036903	0.015517

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0081447567	-0.0677831963	-1.2788296046
C	6.0	-1.2262595097	-0.0266540475	-0.6327846169
C	6.0	1.2093449534	-0.0307652699	-0.5787996417
H	1.0	-1.2073583371	-0.0079211098	0.4473486214
H	1.0	1.1610519862	0.0161998792	0.4998262719
C	6.0	-2.4490560375	-0.0054458568	-1.3034702516
C	6.0	2.4446685557	-0.0276700061	-1.2285459466
C	6.0	-3.6784481112	0.0250978758	-0.6404362614
C	6.0	3.6786729480	0.0174262375	-0.5866323979
N	7.0	-4.8437278194	0.0636551493	-1.3223180997
N	7.0	4.8329726067	0.0683161938	-1.2890862885
C	6.0	-5.9562544765	0.0426664168	-0.4669260077
C	6.0	5.9581388793	0.0452703856	-0.4511368023
C	6.0	-7.3026105449	0.0468753985	-0.8015919386
C	6.0	7.2991566208	0.0552123843	-0.8058100715
H	1.0	-7.6377409961	0.0608189823	-1.8284040114
H	1.0	7.6182337107	0.0774065064	-1.8376511281
C	6.0	-8.2190280176	0.0267345684	0.2490613504
C	6.0	8.2316430898	0.0293100264	0.2308433879
H	1.0	-9.2775534318	0.0288381332	0.0261070284
H	1.0	9.2866668186	0.0347490406	-0.0079539155

C	6.0	-7.7926071678	0.0014601230	1.5743045274
C	6.0	7.8257381820	-0.0057768387	1.5622188030
H	1.0	-8.5227663373	-0.0139751542	2.3719806277
H	1.0	8.5679686047	-0.0256077999	2.3485733403
C	6.0	-6.4290300304	-0.0072296192	1.8839100280
C	6.0	6.4669332862	-0.0188996346	1.8922873508
H	1.0	-6.1089932839	-0.0296096025	2.9175127644
H	1.0	6.1623192011	-0.0487477053	2.9303451267
C	6.0	-5.5105726740	0.0111817541	0.8508008083
C	6.0	5.5327019390	0.0038026815	0.8737526319
C	6.0	-3.9921309020	0.0025597549	0.8670542617
C	6.0	4.0144293499	-0.0063726088	0.9139322938
C	6.0	-3.4625850715	1.2639175642	1.5843105856
C	6.0	3.4912903958	1.2542748078	1.6371197210
C	6.0	-3.4784888229	-1.2859104411	1.5450837842
C	6.0	3.5026171787	-1.2930718922	1.5948740999
H	1.0	-3.8133099515	2.1700469347	1.0909005716
H	1.0	3.8338709437	2.1613146997	1.1397431589
H	1.0	-3.8378623903	-2.1723211050	1.0229227673
H	1.0	3.8596369841	-2.1807457820	1.0733077258
H	1.0	-3.8259731482	1.2738705320	2.6120305279
H	1.0	3.8655280405	1.2650960401	2.6609149662
H	1.0	-3.8447051679	-1.3235852162	2.5710817303
H	1.0	3.8693885014	-1.3300069406	2.6207167352
H	1.0	-2.3751960272	1.2880169606	1.6114254395
H	1.0	2.4040100038	1.2743106191	1.6755446477
H	1.0	-2.3916379596	-1.3227068340	1.5742242043
H	1.0	2.4153893593	-1.3266544324	1.6239319273
C	6.0	-4.9504909884	0.1161825205	-2.7804729763
C	6.0	4.9115595069	0.1320659588	-2.7488525414
C	6.0	0.0583619638	-0.1024035843	-2.7881084162
C	6.0	2.4262820435	-0.0589086670	-2.7513392159
C	6.0	-2.4452036677	-0.0140124816	-2.8299782399
C	6.0	-3.6809638181	0.7013189280	-3.3747989989
C	6.0	-1.1529771936	0.5931492891	-3.3839505600
C	6.0	3.6187134964	0.6873630345	-3.3250737438
O	8.0	1.2418420751	0.5427129961	-3.2617581103
H	1.0	5.1212468682	-0.8691305277	-3.1332271300
H	1.0	5.7516271444	0.7711386530	-3.0138159133
H	1.0	3.6376881139	0.5916671743	-4.4096937093
H	1.0	3.5243343302	1.7468228573	-3.0804958263
H	1.0	2.4601387373	-1.1049269474	-3.0896928082
H	1.0	0.0760317166	-1.1473738191	-3.1308829371
H	1.0	-1.1336086390	0.5014047583	-4.4706697914
H	1.0	-1.1047676413	1.6570346048	-3.1372745523
H	1.0	-2.4923315758	-1.0585091999	-3.1617208226
H	1.0	-3.7262283483	0.6106764988	-4.4600455481
H	1.0	-3.6244034738	1.7661649117	-3.1366141319
H	1.0	-5.1346674596	-0.8935011352	-3.1554143215
H	1.0	-5.8154353509	0.7275325606	-3.0314917879

Conformationally restrained pentamethine indocyanine: Results at TDDFT-B3LYP-PCM/cc-pVTZ excited state optimized structure (S1)

E(S0) = -1462.753801
E(S1) = -1462.684556*
Oscillator strength = 2.1984
E(HOMO) = -0.1910; E(LUMO) = -0.1090

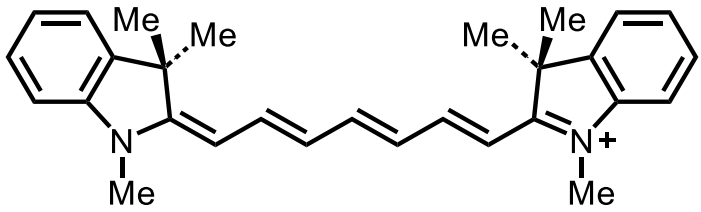
OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
125	128	-0.035865	-0.023452
127	128	0.997743	-0.090280
126	129	-0.079062	-0.022833
126	131	0.032359	0.013451
127	132	0.030927	0.014856

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1208664222	-0.1010835341	-0.5072587914
C	6.0	-1.1060190353	-0.1234365619	-1.1796473950
C	6.0	1.3382085371	-0.1070822070	-1.1968556155
C	6.0	-2.3384415645	-0.1082876574	-0.5232817659
C	6.0	2.5797707178	-0.0756197308	-0.5581185096
H	1.0	-2.3140596734	-0.1060597704	0.5564073058
H	1.0	2.5698840256	-0.0749449529	0.5218555245
C	6.0	-3.5759185090	-0.0915743255	-1.1898979487
C	6.0	3.8072193403	-0.0402552845	-1.2422951218
C	6.0	-4.8039797844	-0.0858911018	-0.5270718258
C	6.0	5.0446544760	-0.0176145300	-0.5973747316
N	7.0	-5.9852534867	-0.0623721883	-1.2170850150
N	7.0	6.2153454871	0.0233746017	-1.3043660411
C	6.0	-7.0829855855	-0.1072697270	-0.3722433918
C	6.0	7.3257718839	-0.0047402317	-0.4755081289
C	6.0	-8.4367930745	-0.1234523985	-0.7042752795
C	6.0	8.6748108401	-0.0020033807	-0.8267371990
H	1.0	-8.7728790262	-0.1105056799	-1.7307455299
H	1.0	8.9957552161	0.0145383834	-1.8579674600
C	6.0	-9.3489985255	-0.1635046630	0.3449633314
C	6.0	9.6024697632	-0.0280073448	0.2094017534
H	1.0	-10.4078696608	-0.1772806741	0.1235064997
H	1.0	10.6581903719	-0.0272301576	-0.0268936481
C	6.0	-8.9223066061	-0.1889195800	1.6731156365
C	6.0	9.1952318209	-0.0577095170	1.5436246425
H	1.0	-9.6530064144	-0.2201943171	2.4697986773
H	1.0	9.9376406639	-0.0774327858	2.3297872034
C	6.0	-7.5577312543	-0.1776355813	1.9835511411
C	6.0	7.8352803307	-0.0659481830	1.8733117129
H	1.0	-7.2389277529	-0.2004718967	3.0175848633

H	1.0	7.5312423528	-0.0924769955	2.9116661820
C	6.0	-6.6383664653	-0.1391861600	0.9541196972
C	6.0	6.9009388265	-0.0421003544	0.8570587061
C	6.0	-5.1207286290	-0.1232924307	0.9749514629
C	6.0	5.3838059339	-0.0500396962	0.8998949666
C	6.0	-4.5886909559	-1.4066078151	1.6540000856
C	6.0	4.8818887318	-1.3416174677	1.5862192613
C	6.0	-4.6115678530	1.1389110105	1.7098329268
C	6.0	4.8652660165	1.2040535304	1.6420916741
H	1.0	-4.9379447504	-2.2973575405	1.1324767317
H	1.0	5.2381358577	-2.2267172426	1.0598358199
H	1.0	-4.9857470237	2.0446491139	1.2333315771
H	1.0	5.2154475096	2.1156121963	1.1585028095
H	1.0	-4.9514064817	-1.4486386101	2.6813934691
H	1.0	5.2590036159	-1.3779442353	2.6086053068
H	1.0	-4.9648008593	1.1255073475	2.7413966079
H	1.0	5.2356869984	1.1980784984	2.6676396355
H	1.0	-3.5013269982	-1.4284148686	1.6795010565
H	1.0	3.7954637600	-1.3805470200	1.6263499590
H	1.0	-3.5245614837	1.1835094074	1.7257828425
H	1.0	3.7780181280	1.2300708671	1.6760015450
H	1.0	0.1279936752	-0.0640508469	0.5766323991
C	6.0	6.2924822198	0.0714554838	-2.7615703122
C	6.0	-6.0831845742	-0.0211397619	-2.6732261992
C	6.0	-3.5770350725	-0.0871837089	-2.7140135901
C	6.0	-1.0769068621	-0.1519138158	-2.6905457047
C	6.0	1.2886265130	-0.1348479639	-2.7071968355
C	6.0	3.7869197626	-0.0333144912	-2.7662857794
C	6.0	-4.8277834550	0.6006347518	-3.2595011740
C	6.0	-2.2966701023	0.5399475988	-3.2709985004
C	6.0	5.0190789940	0.6749337025	-3.3278873028
C	6.0	2.4895953745	0.5757873615	-3.3037609400
O	8.0	0.0978622169	0.4795040025	-3.1940994122
H	1.0	7.1630117427	0.6647548463	-3.0361905668
H	1.0	6.4471126268	-0.9429721463	-3.1409823369
H	1.0	-6.2259312100	-1.0396243623	-3.0464445740
H	1.0	-6.9671241644	0.5563681415	-2.9383965060
H	1.0	-4.7991505092	1.6657154234	-3.0171880834
H	1.0	4.9773004376	1.7387586520	-3.0822247902
H	1.0	5.0423120061	0.5901997473	-4.4144456073
H	1.0	-4.8653188592	0.5124984297	-4.3453560466
H	1.0	-2.2835631390	0.4555715641	-4.3584625101
H	1.0	-2.2573735236	1.6025104837	-3.0172123416
H	1.0	2.4621730247	0.4930528442	-4.3910442761
H	1.0	2.4384959965	1.6372103907	-3.0474808637
H	1.0	3.8234777097	-1.0787343833	-3.1004766884
H	1.0	1.2964736654	-1.1858248349	-3.0387930672
H	1.0	-1.0735602998	-1.2031527354	-3.0212697272
H	1.0	-3.6026630486	-1.1338439098	-3.0455077095

Parent heptamethine indocyanine: Results at B3LYP-PCM/cc-pVTZ ground state optimized structure (S0)



E(S0) = -1233.929417
E(S1) = -1233.852646*
Oscillator strength = 2.6792
E(HOMO) = -0.1898; E(LUMO) = -0.1108

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
108	111	0.065672	0.028473
110	111	1.002232	-0.156535
109	112	0.103635	0.023700
110	115	-0.036216	-0.014286

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1204506943	-0.0839283767	-0.5292279538
C	6.0	-1.1160531975	-0.0911748710	-1.1669097667
C	6.0	1.3472774383	-0.0748238285	-1.1852605833
C	6.0	-2.3244020351	-0.1015345827	-0.4835518021
C	6.0	2.5657289771	-0.0674333084	-0.5200950677
H	1.0	-2.2739473282	-0.1038756612	0.5977936100
H	1.0	2.5306515996	-0.0682201055	0.5619138459
C	6.0	-3.5690361819	-0.1088819894	-1.1134549131
C	6.0	3.8010267276	-0.0592076753	-1.1679990326
H	1.0	-3.5583287696	-0.1049422085	-2.1957595466
H	1.0	3.7754592132	-0.0598814442	-2.2500234959
C	6.0	-4.8127986852	-0.1211095411	-0.4978538988
C	6.0	5.0535637658	-0.0507999102	-0.5703155273
N	7.0	-5.9599038785	-0.1269295846	-1.2158914914
N	7.0	6.1904347994	-0.0401589077	-1.3044819389
C	6.0	-6.0210225228	-0.1202828415	-2.6705402392
C	6.0	6.2305298009	-0.0341401553	-2.7599102715
H	1.0	-7.0579257607	-0.1261481816	-2.9844386450
H	1.0	7.2616554173	0.0114591909	-3.0894847604
H	1.0	-5.5275853967	-1.0034065369	-3.0758172816
H	1.0	5.7742190765	-0.9406811855	-3.1573515356
H	1.0	-5.5402263999	0.7736976209	-3.0670893124
H	1.0	5.7014890968	0.8348945497	-3.1499092058
C	6.0	-7.0938755055	-0.1413058715	-0.3825325937

C	6.0	7.3361527804	-0.0394264842	-0.4871862438
C	6.0	-8.4357376301	-0.1510477620	-0.7362529527
C	6.0	8.6732127431	-0.0345812690	-0.8588097034
H	1.0	-8.7598327850	-0.1481727220	-1.7663765341
H	1.0	8.9833331908	-0.0319993294	-1.8932324549
C	6.0	-9.3710694340	-0.1651439746	0.2975712939
C	6.0	9.6225345841	-0.0342672746	0.1624166060
H	1.0	-10.4249303300	-0.1730302549	0.0537190256
H	1.0	10.6730515191	-0.0306675152	-0.0953690467
C	6.0	-8.9710125373	-0.1692379465	1.6309706628
C	6.0	9.2406609512	-0.0389185889	1.5012129724
H	1.0	-9.7154882104	-0.1803825312	2.4153344974
H	1.0	9.9957006439	-0.0385968334	2.2755010419
C	6.0	-7.6134392972	-0.1589961837	1.9627448289
C	6.0	7.8877864671	-0.0447053328	1.8510408091
H	1.0	-7.3095696238	-0.1621788658	3.0014737140
H	1.0	7.5976093847	-0.0489841868	2.8936564463
C	6.0	-6.6766573378	-0.1449238449	0.9461352360
C	6.0	6.9374394801	-0.0453530649	0.8471506486
C	6.0	-5.1609191677	-0.1312803089	0.9972706456
C	6.0	5.4225550864	-0.0526511422	0.9195484132
C	6.0	-4.6337868376	-1.4030196198	1.6964287292
C	6.0	4.9232777891	-1.3301552177	1.6285986140
C	6.0	-4.6572074159	1.1438005174	1.7077083546
C	6.0	4.9108537125	1.2169701415	1.6340965545
H	1.0	-4.9744133433	-2.3018133132	1.1829545920
H	1.0	5.2700073694	-2.2251680284	1.1126109058
H	1.0	-5.0147790075	2.0406300440	1.2023641264
H	1.0	5.2494732588	2.1175265001	1.1223882940
H	1.0	-5.0054819184	-1.4338768276	2.7207084381
H	1.0	5.3087378288	-1.3534053079	2.6479565908
H	1.0	-5.0289748191	1.1588901112	2.7323383285
H	1.0	5.2954407019	1.2391684453	2.6538095237
H	1.0	-3.5462282496	-1.4198831820	1.7315850205
H	1.0	3.8366321670	-1.3625545116	1.6781186274
H	1.0	-3.5701332891	1.1802490337	1.7426411155
H	1.0	3.8238902409	1.2390137524	1.6828945062
H	1.0	0.1281000312	-0.0856791308	0.5576963778
H	1.0	-1.1351558433	-0.0890087201	-2.2524181365
H	1.0	1.3507712110	-0.0735216443	-2.2709594206

Parent heptamethine indocyanine: Results at TDDFT-B3LYP-PCM/cc-pVTZ excited state optimized structure (S1)

E(S0) = -1233.928031*
E(S1) = -1233.864627
Oscillator strength = 2.8196
E(HOMO) = -0.1904; E(LUMO) = -0.1143

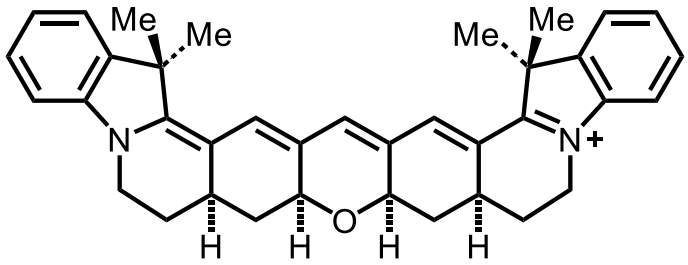
OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
110	111	0.997264	-0.083759
109	112	0.089567	0.025867

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1218201239	-0.0909176396	-0.3777313420
C	6.0	-1.1161453469	-0.0975613411	-1.0231936749
C	6.0	1.3498604672	-0.0823580898	-1.0419286496
C	6.0	-2.3421017804	-0.1064006518	-0.3631526034
C	6.0	2.5855821392	-0.0735905133	-0.4003952767
H	1.0	-2.3197255065	-0.1088387026	0.7184411347
H	1.0	2.5785451417	-0.0733282317	0.6813852715
C	6.0	-3.5734019173	-0.1117845924	-1.0339242009
C	6.0	3.8067427606	-0.0640852826	-1.0894335913
H	1.0	-3.5258954388	-0.1073706844	-2.1160663559
H	1.0	3.7429745276	-0.0654798201	-2.1707553001
C	6.0	-4.8376958262	-0.1222547919	-0.4660123424
C	6.0	5.0791084635	-0.0529985364	-0.5399125831
N	7.0	-5.9725293985	-0.1255447081	-1.2345039693
N	7.0	6.2032732895	-0.0400700034	-1.3238693116
C	6.0	-5.9744546698	-0.1170036405	-2.6880192531
C	6.0	6.1846365197	-0.0328629674	-2.7772249234
H	1.0	-6.9961592101	-0.1175388493	-3.0491586804
H	1.0	7.1999556633	0.0158144561	-3.1529839482
H	1.0	-5.4659417610	-1.0013823322	-3.0736174870
H	1.0	5.7125450797	-0.9401726652	-3.1563779612
H	1.0	-5.4709937596	0.7748597406	-3.0626972243
H	1.0	5.6346557732	0.8342224884	-3.1437724919
C	6.0	-7.1203193911	-0.1386981208	-0.4518220075
C	6.0	7.3617498424	-0.0371159895	-0.5569284995
C	6.0	-8.4574889277	-0.1467759286	-0.8489300096
C	6.0	8.6935454248	-0.0299969471	-0.9716537321
H	1.0	-8.7465593218	-0.1433285637	-1.8893478427
H	1.0	8.9689614681	-0.0275425236	-2.0158283921
C	6.0	-9.4234331933	-0.1599298044	0.1509395767
C	6.0	9.6727056039	-0.0275394342	0.0154356990
H	1.0	-10.4689505522	-0.1664962033	-0.1263160832
H	1.0	10.7144368067	-0.0221356156	-0.2755870227

C	6.0	-9.0692276851	-0.1649584156	1.5011085740
C	6.0	9.3364160828	-0.0323077252	1.3702705132
H	1.0	-9.8411165314	-0.1752999282	2.2584544576
H	1.0	10.1182630429	-0.0301668168	2.1173868719
C	6.0	-7.7237534380	-0.1567325367	1.8803227836
C	6.0	7.9962198763	-0.0405720272	1.7671447821
H	1.0	-7.4569279109	-0.1608240909	2.9291769837
H	1.0	7.7433083215	-0.0448287474	2.8194873779
C	6.0	-6.7520048399	-0.1436178381	0.9000789927
C	6.0	7.0116783933	-0.0434392456	0.7998615862
C	6.0	-5.2409226087	-0.1327006925	1.0100212557
C	6.0	5.5021876425	-0.0530281414	0.9303465160
C	6.0	-4.7433920430	-1.4047140174	1.7350556698
C	6.0	5.0325353269	-1.3289563378	1.6669808225
C	6.0	-4.7626151794	1.1395172463	1.7476629373
C	6.0	5.0166812780	1.2154376906	1.6699885947
H	1.0	-5.0739880964	-2.3043311112	1.2166836945
H	1.0	5.3675889049	-2.2259732723	1.1469905847
H	1.0	-5.1052233109	2.0391330979	1.2371317411
H	1.0	5.3424604673	2.1177445811	1.1532590872
H	1.0	-5.1445346163	-1.4268372871	2.7485897992
H	1.0	5.4486398469	-1.3421101695	2.6746271389
H	1.0	-5.1655083560	1.1466769358	2.7607335561
H	1.0	5.4308032117	1.2302104839	2.6784250799
H	1.0	-3.6573144588	-1.4265898935	1.8012319780
H	1.0	3.9479593827	-1.3653287221	1.7495103454
H	1.0	-3.6770489610	1.1760227909	1.8158776346
H	1.0	3.9315662787	1.2392377801	1.7502929104
H	1.0	0.1296967450	-0.0920291063	0.7083368953
H	1.0	-1.1219656866	-0.0956460732	-2.1097679381
H	1.0	1.3400208364	-0.0819797008	-2.1284785070

Conformationally restrained heptamethine indocyanine: Results at B3LYP-PCM/cc-pVTZ ground state optimized structure (S0)



E(S0) = -1617.539846
E(S1) = -1617.467141*
Oscillator strength = 2.4005
E(HOMO) = -0.1823; E(LUMO) = -0.1079

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
139	142	0.053893	0.024613
141	142	-1.005217	0.168146
140	143	0.097910	0.025190
141	146	0.033313	0.014891

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1202111649	-0.1992484611	-0.5824022723
C	6.0	-1.1013152766	-0.2103184851	-1.2517102110
C	6.0	1.3330189557	-0.1975792060	-1.2677828579
C	6.0	-2.3201696534	-0.1710559916	-0.5819702487
C	6.0	2.5602681308	-0.1401567859	-0.6149831116
H	1.0	-2.2804868222	-0.1747080633	0.4976707871
H	1.0	2.5345244593	-0.1359969494	0.4651789944
C	6.0	-3.5589479387	-0.1240823997	-1.2274487805
C	6.0	3.7899133949	-0.0852847337	-1.2776247942
C	6.0	-4.7718003744	-0.0945107034	-0.5397976180
C	6.0	5.0117946117	-0.0318775600	-0.6077928188
N	7.0	-5.9536599033	-0.0262620572	-1.1960390150
N	7.0	6.1836162270	0.0363349381	-1.2822419258
C	6.0	-7.0460508886	-0.0558117933	-0.3174093631
C	6.0	7.2885022983	0.0403238360	-0.4192029834
C	6.0	-8.4000937836	-0.0267309519	-0.6200116173
C	6.0	8.6375207567	0.0780494383	-0.7425225996
H	1.0	-8.7593276533	0.0185297205	-1.6378666611
H	1.0	8.9806153186	0.1025012036	-1.7665667109
C	6.0	-9.2928041112	-0.0629266360	0.4506671888
C	6.0	9.5462065579	0.0785294708	0.3151944654
H	1.0	-10.3559943576	-0.0425208373	0.2517879893

H	1.0	10.6060600117	0.1067548271	0.1001174977
C	6.0	-8.8372877264	-0.1280422378	1.7647712882
C	6.0	9.1107125327	0.0404906977	1.6370998569
H	1.0	-9.5492561700	-0.1557903863	2.5784203795
H	1.0	9.8347264367	0.0417171832	2.4405329252
C	6.0	-7.4670809597	-0.1604127358	2.0423830620
C	6.0	7.7451379365	-0.0026451185	1.9356804524
H	1.0	-7.1239478526	-0.2133706030	3.0675598564
H	1.0	7.4175821237	-0.0353652903	2.9667300916
C	6.0	-6.5720633132	-0.1258301848	0.9896698968
C	6.0	6.8344072354	-0.0049189347	0.8958672176
C	6.0	-5.0534535476	-0.1493369058	0.9729510990
C	6.0	5.3163793274	-0.0524173786	0.9018251244
C	6.0	-4.5377988012	-1.4564363068	1.6123298332
C	6.0	4.8320551470	-1.3562097797	1.5723450964
C	6.0	-4.4982031793	1.0906937194	1.7082302271
C	6.0	4.7496011318	1.1910557341	1.6216295014
H	1.0	-4.9151239060	-2.3281478279	1.0781974784
H	1.0	5.2166373642	-2.2311902594	1.0488287688
H	1.0	-4.8562726154	2.0107457625	1.2467659877
H	1.0	5.0776608796	2.1084405671	1.1333609809
H	1.0	-4.8842172276	-1.5133419321	2.6443696466
H	1.0	5.1934626666	-1.3890819611	2.6003142624
H	1.0	-4.8354443963	1.0768997070	2.7448917109
H	1.0	5.1073711084	1.2071099870	2.6513408290
H	1.0	-3.4509471777	-1.5025305284	1.6193384447
H	1.0	3.7463333199	-1.4200214395	1.5953297170
H	1.0	-3.4103242891	1.1086732819	1.7081331444
H	1.0	3.6617562953	1.1854131892	1.6432810310
H	1.0	0.1267730034	-0.1684086538	0.5024980110
C	6.0	6.2972028432	0.0958981778	-2.7387778103
C	6.0	-6.0887970970	0.0627724640	-2.6493933611
C	6.0	-3.5855165095	-0.1004914731	-2.7533531727
C	6.0	-1.0807988499	-0.2202960224	-2.7649943355
C	6.0	1.2906352127	-0.2139799607	-2.7806017002
C	6.0	3.7939853340	-0.0810023494	-2.8041345872
C	6.0	-4.8226714224	0.6431368118	-3.2564990275
C	6.0	-2.2964680502	0.5007838201	-3.3218192473
C	6.0	5.0198680803	0.6596102912	-3.3376975364
C	6.0	2.4942341873	0.5090491547	-3.3596583005
O	8.0	0.0998551372	0.4106299942	-3.2625482262
H	1.0	7.1516640278	0.7243596521	-2.9838699766
H	1.0	6.5024363580	-0.9084997631	-3.1177032176
H	1.0	-6.2962957157	-0.9345436870	-3.0453688343
H	1.0	-6.9490509627	0.6928755893	-2.8689950476
H	1.0	-4.7454628082	1.7011195665	-2.9945362119
H	1.0	4.9417324365	1.7217751310	-3.0936352352
H	1.0	5.0729552634	0.5763394879	-4.4232061452
H	1.0	-4.8915375997	0.5792022640	-4.3423626957
H	1.0	-2.3006910598	0.4304281354	-4.4103800420
H	1.0	-2.2297062707	1.5590388721	-3.0556059388
H	1.0	2.4837662607	0.4298008171	-4.4475653398

H	1.0	2.4258610728	1.5691040910	-3.1012677564
H	1.0	3.8595177710	-1.1217901760	-3.1443932540
H	1.0	1.2977612820	-1.2569768558	-3.1314843065
H	1.0	-1.0896753258	-1.2618933091	-3.1201044522
H	1.0	-3.6532427468	-1.1370068877	-3.1059553255

Conformationally restrained heptamethine indocyanine: Results at TDDFT-B3LYP-PCM/cc-pVTZ excited state optimized structure (S1)

E(S0) = -1617.538648
E(S1) = -1617.478241*
Oscillator strength = 2.6624
E(HOMO) = -0.1829; E(LUMO) = -0.1111

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
139	142	-0.032261	-0.021974
141	142	0.998434	-0.097087
140	143	0.087801	0.028019

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1208664222	-0.1010835341	-0.5072587914
C	6.0	-1.1060190353	-0.1234365619	-1.1796473950
C	6.0	1.3382085371	-0.1070822070	-1.1968556155
C	6.0	-2.3384415645	-0.1082876574	-0.5232817659
C	6.0	2.5797707178	-0.0756197308	-0.5581185096
H	1.0	-2.3140596734	-0.1060597704	0.5564073058
H	1.0	2.5698840256	-0.0749449529	0.5218555245
C	6.0	-3.5759185090	-0.0915743255	-1.1898979487
C	6.0	3.8072193403	-0.0402552845	-1.2422951218
C	6.0	-4.8039797844	-0.0858911018	-0.5270718258
C	6.0	5.0446544760	-0.0176145300	-0.5973747316
N	7.0	-5.9852534867	-0.0623721883	-1.2170850150
N	7.0	6.2153454871	0.0233746017	-1.3043660411
C	6.0	-7.0829855855	-0.1072697270	-0.3722433918
C	6.0	7.3257718839	-0.0047402317	-0.4755081289
C	6.0	-8.4367930745	-0.1234523985	-0.7042752795
C	6.0	8.6748108401	-0.0020033807	-0.8267371990
H	1.0	-8.7728790262	-0.1105056799	-1.7307455299
H	1.0	8.9957552161	0.0145383834	-1.8579674600
C	6.0	-9.3489985255	-0.1635046630	0.3449633314
C	6.0	9.6024697632	-0.0280073448	0.2094017534
H	1.0	-10.4078696608	-0.1772806741	0.1235064997
H	1.0	10.6581903719	-0.0272301576	-0.0268936481
C	6.0	-8.9223066061	-0.1889195800	1.6731156365
C	6.0	9.1952318209	-0.0577095170	1.5436246425
H	1.0	-9.6530064144	-0.2201943171	2.4697986773
H	1.0	9.9376406639	-0.0774327858	2.3297872034
C	6.0	-7.5577312543	-0.1776355813	1.9835511411
C	6.0	7.8352803307	-0.0659481830	1.8733117129
H	1.0	-7.2389277529	-0.2004718967	3.0175848633
H	1.0	7.5312423528	-0.0924769955	2.9116661820
C	6.0	-6.6383664653	-0.1391861600	0.9541196972

C	6.0	6.9009388265	-0.0421003544	0.8570587061
C	6.0	-5.1207286290	-0.1232924307	0.9749514629
C	6.0	5.3838059339	-0.0500396962	0.8998949666
C	6.0	-4.5886909559	-1.4066078151	1.6540000856
C	6.0	4.8818887318	-1.3416174677	1.5862192613
C	6.0	-4.6115678530	1.1389110105	1.7098329268
C	6.0	4.8652660165	1.2040535304	1.6420916741
H	1.0	-4.9379447504	-2.2973575405	1.1324767317
H	1.0	5.2381358577	-2.2267172426	1.0598358199
H	1.0	-4.9857470237	2.0446491139	1.2333315771
H	1.0	5.2154475096	2.1156121963	1.1585028095
H	1.0	-4.9514064817	-1.4486386101	2.6813934691
H	1.0	5.2590036159	-1.3779442353	2.6086053068
H	1.0	-4.9648008593	1.1255073475	2.7413966079
H	1.0	5.2356869984	1.1980784984	2.6676396355
H	1.0	-3.5013269982	-1.4284148686	1.6795010565
H	1.0	3.7954637600	-1.3805470200	1.6263499590
H	1.0	-3.5245614837	1.1835094074	1.7257828425
H	1.0	3.7780181280	1.2300708671	1.6760015450
H	1.0	0.1279936752	-0.0640508469	0.5766323991
C	6.0	6.2924822198	0.0714554838	-2.7615703122
C	6.0	-6.0831845742	-0.0211397619	-2.6732261992
C	6.0	-3.5770350725	-0.0871837089	-2.7140135901
C	6.0	-1.0769068621	-0.1519138158	-2.6905457047
C	6.0	1.2886265130	-0.1348479639	-2.7071968355
C	6.0	3.7869197626	-0.0333144912	-2.7662857794
C	6.0	-4.8277834550	0.6006347518	-3.2595011740
C	6.0	-2.2966701023	0.5399475988	-3.2709985004
C	6.0	5.0190789940	0.6749337025	-3.3278873028
C	6.0	2.4895953745	0.5757873615	-3.3037609400
O	8.0	0.0978622169	0.4795040025	-3.1940994122
H	1.0	7.1630117427	0.6647548463	-3.0361905668
H	1.0	6.4471126268	-0.9429721463	-3.1409823369
H	1.0	-6.2259312100	-1.0396243623	-3.0464445740
H	1.0	-6.9671241644	0.5563681415	-2.9383965060
H	1.0	-4.7991505092	1.6657154234	-3.0171880834
H	1.0	4.9773004376	1.7387586520	-3.0822247902
H	1.0	5.0423120061	0.5901997473	-4.4144456073
H	1.0	-4.8653188592	0.5124984297	-4.3453560466
H	1.0	-2.2835631390	0.4555715641	-4.3584625101
H	1.0	-2.2573735236	1.6025104837	-3.0172123416
H	1.0	2.4621730247	0.4930528442	-4.3910442761
H	1.0	2.4384959965	1.6372103907	-3.0474808637
H	1.0	3.8234777097	-1.0787343833	-3.1004766884
H	1.0	1.2964736654	-1.1858248349	-3.0387930672
H	1.0	-1.0735602998	-1.2031527354	-3.0212697272
H	1.0	-3.6026630486	-1.1338439098	-3.0455077095

Section S6. Raw ORMAS-PT2-PCM/6-31G(d) Results: Absolute energies (hartree) and geometries (Å)

Parent trimethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at B3LYP-PCM/6-31G(d) ground state optimized structure (S0)

E(S0) = -1075.913573
E(S1) = -1075.825042*

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.0000720793	-0.0007505815	0.5514343184
H	1.0	-0.0001195910	-0.0005935117	-0.5313460857
C	6.0	-1.2260152897	0.0053807762	1.2224636028
C	6.0	1.2259852617	-0.0069528233	1.2222911828
H	1.0	-1.1833212790	0.0039062668	2.3079868139
H	1.0	1.1832559755	-0.0059878323	2.3077942298
C	6.0	-2.4942538058	0.0114321315	0.6368849531
C	6.0	2.4942305804	-0.0119995848	0.6367674356
N	7.0	-3.6219405890	0.0276032936	1.3886109853
N	7.0	3.6218540244	-0.0275497097	1.3886975873
C	6.0	-3.6392827683	0.0502265653	2.8492303341
C	6.0	3.6387765777	-0.0512806157	2.8493084161
H	1.0	-4.6669112537	0.1432798484	3.1950019596
H	1.0	4.6665216677	-0.1408496313	3.1955772734
H	1.0	-3.2108415798	-0.8738523199	3.2496215157
H	1.0	3.0696800616	-0.9097102098	3.2171593352
H	1.0	-3.0672826217	0.9063055302	3.2180135365
H	1.0	3.2069460849	0.8709730953	3.2502509759
C	6.0	-4.7856851611	0.0145675147	0.5847544627
C	6.0	4.7856811509	-0.0135415750	0.5849845372
C	6.0	-6.1222161703	0.0144263462	0.9770004756
C	6.0	6.1221646242	-0.0125201751	0.9774267689
H	1.0	-6.4206485172	0.0216049804	2.0197067201
H	1.0	6.4203505964	-0.0197516199	2.0201927264
C	6.0	-7.0878746893	0.0012130161	-0.0370844610
C	6.0	7.0880180136	0.0013967118	-0.0364588249
H	1.0	-8.1393304226	0.0004691117	0.2356105196
H	1.0	8.1394210085	0.0027465390	0.2364878923
C	6.0	-6.7213807776	-0.0120171557	-1.3870466248
C	6.0	6.7217145969	0.0144984575	-1.3864633954
H	1.0	-7.4893171309	-0.0221882184	-2.1550515708
H	1.0	7.4897818058	0.0251731628	-2.1543330473
C	6.0	-5.3683583389	-0.0135462258	-1.7566442146
C	6.0	5.3687420888	0.0151974166	-1.7563355076
H	1.0	-5.0879398162	-0.0252596357	-2.8066152655
H	1.0	5.0886294880	0.0267549276	-2.8063889226
C	6.0	-4.4020380028	-0.0011018843	-0.7593765570
C	6.0	4.4022353451	0.0020448898	-0.7592229747
C	6.0	-2.8845682488	-0.0022503238	-0.8509577082
C	6.0	2.8847686919	0.0022420065	-0.8510111618

C	6.0	2.3911559172	1.2876436839	-1.5593899800
C	6.0	-2.3907420968	1.2706565909	-1.5820818507
C	6.0	2.3917645688	-1.2709109687	-1.5822563746
C	6.0	-2.3915439069	-1.2878190273	-1.5594765800
H	1.0	2.7309710439	2.1836555069	-1.0306399675
H	1.0	-2.7306174450	2.1759595390	-1.0694538230
H	1.0	2.7315553624	-2.1760151691	-1.0691951350
H	1.0	-2.7324702720	-2.1837832804	-1.0313739202
H	1.0	2.7901718315	1.3181156793	-2.5785385266
H	1.0	-2.7896724971	1.2830844388	-2.6016692895
H	1.0	2.7913376544	-1.2834752322	-2.6015872662
H	1.0	-2.7898603722	-1.3175772120	-2.5789183756
H	1.0	1.2999687206	1.3224305951	-1.6247745891
H	1.0	-1.2995114089	1.3042963746	-1.6478438429
H	1.0	1.3005747812	-1.3047625909	-1.6487283003
H	1.0	-1.3003417925	-1.3235592723	-1.6240076552

Parent trimethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at TDDFT-B3LYP-PCM/6-31G(d) excited state optimized structure (S1)

E(S0) = -1075.908131*
E(S1) = -1075.827431

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.0000056884	-0.0009395788	0.4406503364
H	1.0	-0.0000315707	-0.0015321189	-0.6413017650
C	6.0	-1.2295689765	0.0057339534	1.1319828436
C	6.0	1.2294710481	-0.0067538340	1.1321306576
H	1.0	-1.1600269255	0.0087939819	2.2175070496
H	1.0	1.1596051406	-0.0088511281	2.2176092520
C	6.0	-2.5085910172	0.0084743982	0.5871319931
C	6.0	2.5086338747	-0.0093645143	0.5875528282
N	7.0	-3.6422092389	0.0210215424	1.3934424780
N	7.0	3.6422197297	-0.0210627823	1.3939878247
C	6.0	-3.6020302757	0.0390654928	2.8485036646
C	6.0	3.6018553109	-0.0397012320	2.8490444179
H	1.0	-4.6160053053	0.0771985021	3.2427268719
H	1.0	4.6155127041	-0.0840525838	3.2433703706
H	1.0	-3.1090817225	-0.8633128426	3.2271521533
H	1.0	3.0488808783	-0.9175684692	3.2000192857
H	1.0	-3.0543606915	0.9199499745	3.2003342750
H	1.0	3.1138600909	0.8652062354	3.2282733953
C	6.0	-4.7998130087	0.0136353420	0.6380816144
C	6.0	4.7998790294	-0.0121957221	0.6386847156
C	6.0	-6.1395200795	0.0173734979	1.0635238063
C	6.0	6.1397032982	-0.0139399430	1.0639549110
H	1.0	-6.4086996859	0.0257611747	2.1139840473
H	1.0	6.4092008375	-0.0213755419	2.1143264218
C	6.0	-7.1257338313	0.0080412016	0.0799193144
C	6.0	7.1257549870	-0.0038379572	0.0801414328
H	1.0	-8.1702074361	0.0104630856	0.3779723450
H	1.0	8.1703416241	-0.0047315490	0.3779113824
C	6.0	-6.7965978678	-0.0048869223	-1.2868538743
C	6.0	6.7965468205	0.0080299665	-1.2866437257
H	1.0	-7.5875794848	-0.0119032634	-2.0309344340
H	1.0	7.5874191538	0.0156811565	-2.0308391886
C	6.0	-5.4537809214	-0.0092894618	-1.6967036095
C	6.0	5.4536845667	0.0106803872	-1.6962687333
H	1.0	-5.2068586908	-0.0197798536	-2.7550606171
H	1.0	5.2062796943	0.0204751635	-2.7544906723
C	6.0	-4.4578632485	-0.0003443360	-0.7341937294
C	6.0	4.4579438212	0.0010436835	-0.7335967711
C	6.0	-2.9463583889	-0.0028595007	-0.8798138697
C	6.0	2.9465052202	0.0020015476	-0.8792828037
C	6.0	2.4771169200	1.2831770108	-1.6191409583
C	6.0	-2.4760438473	1.2666120141	-1.6394666296

C	6.0	2.4775313719	-1.2682439269	-1.6384159902
C	6.0	-2.4778384481	-1.2844756177	-1.6195107558
H	1.0	2.8076194976	2.1836856808	-1.0921604717
H	1.0	-2.8051236377	2.1755628921	-1.1263027400
H	1.0	2.8073783459	-2.1765278507	-1.1245289102
H	1.0	-2.8088720278	-2.1848190214	-1.0926104305
H	1.0	2.8980298353	1.3008657505	-2.6302533940
H	1.0	-2.8976382654	1.2691269790	-2.6504589265
H	1.0	2.8994251807	-1.2710203795	-2.6492821006
H	1.0	-2.8986793944	-1.3019197373	-2.6306590068
H	1.0	1.3874282558	1.3186115410	-1.7073923421
H	1.0	-1.3863340926	1.2994066214	-1.7289303824
H	1.0	1.3878830005	-1.3021382928	-1.7281577987
H	1.0	-1.3881568695	-1.3205722060	-1.7076782975

Conformationally restrained trimethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at B3LYP-PCM/6-31G(d) ground state optimized structure (S0)

E(S0) = -1304.133837
E(S1) = -1304.047796*

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0008166425	-0.0054500465	0.6180144095
H	1.0	0.0007352187	-0.0659593140	-0.4612330619
C	6.0	-1.2236875377	0.0186581811	1.2955270012
C	6.0	1.2255232447	0.0214678347	1.2952769965
C	6.0	-2.4764760165	-0.0165194543	0.6693601379
C	6.0	2.4781057235	-0.0148154590	0.6689228133
N	7.0	-3.6201083197	-0.0448669782	1.3955536357
N	7.0	3.6221106600	-0.0369487017	1.3949127140
C	6.0	-4.7666151367	-0.0177580026	0.5754041751
C	6.0	4.7683030156	-0.0151721515	0.5742514637
C	6.0	-6.1056458671	-0.0095792551	0.9570969852
C	6.0	6.1075162605	-0.0041075052	0.9552882847
H	1.0	-6.4077831320	-0.0160031696	1.9990301168
H	1.0	6.4100214696	-0.0031405232	1.9971172031
C	6.0	-7.0591049659	0.0150039846	-0.0685580779
C	6.0	7.0606497838	0.0129298973	-0.0707900046
H	1.0	-8.1141283089	0.0228791087	0.1899031472
H	1.0	8.1157275714	0.0225565494	0.1874336887
C	6.0	-6.6744006292	0.0318102581	-1.4136075467
C	6.0	6.6754792183	0.0200607527	-1.4157629586
H	1.0	-7.4331132398	0.0509139718	-2.1905860771
H	1.0	7.4339068438	0.0335604516	-2.1931297621
C	6.0	-5.3167911424	0.0269416363	-1.7697823913
C	6.0	5.3177182307	0.0126275182	-1.7714245540
H	1.0	-5.0264902946	0.0421277308	-2.8169844557
H	1.0	5.0272310230	0.0202251283	-2.8186627670
C	6.0	-4.3619379302	0.0049670685	-0.7618359738
C	6.0	4.3631764558	-0.0022803056	-0.7630219313
C	6.0	-2.8410556413	-0.0038043788	-0.8281654000
C	6.0	2.8422572657	-0.0113630375	-0.8288173515
C	6.0	2.3307520782	1.2646220697	-1.5401843730
C	6.0	-2.3290023624	1.2757885953	-1.5323891078
C	6.0	2.3499882811	-1.2948843959	-1.5428438334
C	6.0	-2.3496349991	-1.2836035458	-1.5496710189
H	1.0	2.6729742335	2.1671027624	-1.0241853336
H	1.0	-2.6717703200	2.1755988560	-1.0121196149
H	1.0	2.6972103505	-2.1926920566	-1.0220517185
H	1.0	-2.6976744628	-2.1841779626	-1.0342501636
H	1.0	2.7151348148	1.2885820253	-2.5651362160
H	1.0	-2.7123277716	1.3049342432	-2.5575990981
H	1.0	2.7443508943	-1.3162471339	-2.5640761197
H	1.0	-2.7439131566	-1.2986295623	-2.5710522284

H	1.0	1.2386942202	1.2929991219	-1.5903141949
H	1.0	-1.2368932296	1.3044886469	-1.5811131497
H	1.0	1.2588575463	-1.3353277596	-1.6041052196
H	1.0	-1.2585459229	-1.3247125889	-1.6110498568
C	6.0	3.6775822471	-0.0755135784	2.8613795946
C	6.0	1.1828192944	0.0754576333	2.8193612574
C	6.0	-1.1824069047	0.0675326603	2.8198282060
C	6.0	-3.6762889374	-0.0998184665	2.8614699519
C	6.0	-2.3753647717	-0.6685763661	3.4200936994
C	6.0	2.3805999942	-0.6484744394	3.4246303576
O	8.0	0.0022638353	-0.5498219058	3.3120977639
H	1.0	4.5285543267	-0.6977145963	3.1493832495
H	1.0	3.8622452485	0.9405875340	3.2311045833
H	1.0	2.3061885027	-1.7162380288	3.1893247477
H	1.0	2.3784287912	-0.5395381288	4.5130359357
H	1.0	1.1895074649	1.1290875800	3.1484054274
H	1.0	-4.5225578946	-0.7321356274	3.1415431132
H	1.0	-3.8698850784	0.9103708323	3.2425117842
H	1.0	-2.2940397008	-1.7340493250	3.1768668559
H	1.0	-2.3737232508	-0.5676405123	4.5092754099
H	1.0	-1.1986594454	1.1199206802	3.1527579505

Conformationally restrained trimethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at TDDFT-B3LYP-PCM/6-31G(d) excited state optimized structure (S1)

E(S0) = -1304.129094*
E(S1) = -1304.049637

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0006374074	-0.0421266796	0.5695517172
H	1.0	0.0005128640	-0.1022603638	-0.5089235339
C	6.0	-1.2341746503	-0.0142033489	1.2559476479
C	6.0	1.2355207561	-0.0166723519	1.2555444821
C	6.0	-2.4921266363	-0.0266665401	0.6463839773
C	6.0	2.4934498787	-0.0284237868	0.6456237419
N	7.0	-3.6533127807	-0.0381662348	1.4066318721
N	7.0	3.6546683140	-0.0448067279	1.4056411357
C	6.0	-4.7838375885	-0.0061296802	0.6163272970
C	6.0	4.7850498604	-0.0081681349	0.6153288584
C	6.0	-6.1318131635	0.0158113944	1.0096780629
C	6.0	6.1330155400	0.0118572514	1.0087773581
H	1.0	-6.4222460496	0.0208187203	2.0547658208
H	1.0	6.4231796776	0.0109948786	2.0539283469
C	6.0	-7.0899947773	0.0396113908	-0.0021378837
C	6.0	7.0912502530	0.0415637667	-0.0028085105
H	1.0	-8.1427922393	0.0576030320	0.2647325006
H	1.0	8.1440036569	0.0584111984	0.2643754125
C	6.0	-6.7205038146	0.0442725164	-1.3581804925
C	6.0	6.7217073920	0.0536499220	-1.3587689806
H	1.0	-7.4899566671	0.0636617829	-2.1243423012
H	1.0	7.4911879053	0.0775206046	-2.1247812597
C	6.0	-5.3663922159	0.0269672906	-1.7324185761
C	6.0	5.3675809263	0.0381151599	-1.7331880821
H	1.0	-5.0917260138	0.0329681234	-2.7838833657
H	1.0	5.0930660026	0.0498187355	-2.7846414330
C	6.0	-4.3977704767	0.0042637489	-0.7422994737
C	6.0	4.3989305754	0.0098804092	-0.7431747868
C	6.0	-2.8800807972	-0.0185858909	-0.8371777238
C	6.0	2.8812223673	-0.0127313606	-0.8379241305
C	6.0	2.3700292579	1.2598967555	-1.5639322116
C	6.0	-2.3693162671	1.2504234293	-1.5699263585
C	6.0	2.4133427459	-1.2926662552	-1.5825954742
C	6.0	-2.4118356610	-1.3021050104	-1.5753733836
H	1.0	2.7008257237	2.1660605725	-1.0470402519
H	1.0	-2.6997770469	2.1592515352	-1.0575467532
H	1.0	2.7636897725	-2.1942916724	-1.0706448453
H	1.0	-2.7631795181	-2.2012645357	-1.0598058023
H	1.0	2.7630689091	1.2827727438	-2.5860372505
H	1.0	-2.7629189973	1.2680776915	-2.5919222451
H	1.0	2.8184058224	-1.2944935471	-2.6003301078
H	1.0	-2.8155757466	-1.3083965189	-2.5936201703

H	1.0	1.2780945885	1.2786714233	-1.6226207338
H	1.0	-1.2774194061	1.2689626316	-1.6293648765
H	1.0	1.3230987722	-1.3414471435	-1.6550554043
H	1.0	-1.3215294394	-1.3516973775	-1.6460812569
C	6.0	3.6733002847	-0.0706556091	2.8689563419
C	6.0	1.1808114431	0.0294360374	2.7781672826
C	6.0	-1.1780071959	0.0352172370	2.7784429578
C	6.0	-3.6708941630	-0.0533002383	2.8700728965
C	6.0	-2.3789459712	-0.6659484916	3.4035868498
C	6.0	2.3787407004	-0.6801988427	3.3996987320
O	8.0	0.0000118494	-0.5974323329	3.2628658148
H	1.0	4.5383635867	-0.6556220480	3.1918717309
H	1.0	3.8031261028	0.9551391876	3.2408418588
H	1.0	2.3314838065	-1.7472041073	3.1542127063
H	1.0	2.3504364294	-0.5797040096	4.4886133400
H	1.0	1.1786773074	1.0868195581	3.1012153724
H	1.0	-4.5387257027	-0.6312823216	3.1979186410
H	1.0	-3.7949293361	0.9759769688	3.2342295923
H	1.0	-2.3365718202	-1.7343066938	3.1631312892
H	1.0	-2.3498950604	-0.5605192201	4.4920249828
H	1.0	-1.1688368968	1.0932204281	3.0991181390

Parent pentamethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at B3LYP-PCM/6-31G(d) ground state optimized structure (S0)

E(S0) = -1153.054405
E(S1) = -1152.977672*

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000249895	0.0000057691	-1.2171622622
H	1.0	-0.0000423590	0.0000039732	-2.3068400212
C	6.0	-1.2248715853	0.0000077208	-0.5480106122
C	6.0	1.2250553721	0.0000046925	-0.5481961016
H	1.0	-1.1906512972	0.0000085008	0.5383239010
H	1.0	1.1909131901	0.0000074279	0.5381369072
C	6.0	-2.4641536855	0.0000088693	-1.1983777432
C	6.0	2.4642303216	-0.0000009197	-1.1987176656
H	1.0	-2.4394031669	0.0000094849	-2.2847333237
H	1.0	2.4393738225	-0.0000044081	-2.2850529676
C	6.0	-3.7199901825	0.0000068027	-0.5918170071
C	6.0	3.7201200223	-0.0000025682	-0.5922121561
N	7.0	-4.8640630794	0.0000154696	-1.3235352893
N	7.0	4.8642210092	-0.0000153804	-1.3238482537
C	6.0	-4.9071809667	0.0000372600	-2.7828389096
C	6.0	4.9073491037	-0.0000340182	-2.7831769157
H	1.0	-5.9444316750	0.0000833784	-3.1119130059
H	1.0	5.9446180727	-0.0000739389	-3.1122109781
H	1.0	-4.4123830266	0.8929977720	-3.1770778474
H	1.0	4.4126526364	0.8929576536	-3.1774466652
H	1.0	-4.4124515402	-0.8929482057	-3.1771056465
H	1.0	4.4125926747	-0.8930032613	-3.1774232753
C	6.0	-6.0105913580	0.0000014057	-0.4977769392
C	6.0	6.0107550101	-0.0000083186	-0.4980034081
C	6.0	-7.3546686289	-0.0000007647	-0.8645925755
C	6.0	7.3549259034	-0.0000142080	-0.8645438273
H	1.0	-7.6723801138	0.0000054174	-1.9016560999
H	1.0	7.6730497715	-0.0000229384	-1.9014712170
C	6.0	-8.3015722646	-0.0000135828	0.1669613404
C	6.0	8.3015759632	-0.0000072613	0.1672651940
H	1.0	-9.3578742002	-0.0000155037	-0.0868108313
H	1.0	9.3579595979	-0.0000118587	-0.0861420825
C	6.0	-7.9103431263	-0.0000245263	1.5098770887
C	6.0	7.9100899888	0.0000057476	1.5101197534
H	1.0	-8.6640389732	-0.0000344021	2.2919704571
H	1.0	8.6636444841	0.0000108451	2.2923573727
C	6.0	-6.5502526868	-0.0000235885	1.8541689412
C	6.0	6.5499564985	0.0000127284	1.8541025601
H	1.0	-6.2508241730	-0.0000327886	2.8990026024
H	1.0	6.2501306977	0.0000233311	2.8988151224
C	6.0	-5.6017596370	-0.0000108853	0.8397185013
C	6.0	5.6017244018	0.0000057994	0.8394351852

C	6.0	-4.0825757406	-0.0000067388	0.9030877048
C	6.0	4.0825641641	0.0000107182	0.9026924212
C	6.0	-3.5725172978	1.2781615978	1.6137935556
C	6.0	3.5724148528	1.2781356155	1.6134201011
C	6.0	-3.5725090643	-1.2781824556	1.6137735446
C	6.0	3.5724073332	-1.2780966822	1.6134464706
H	1.0	-3.9221529216	2.1794846390	1.1002695515
H	1.0	3.9221411586	2.1795327539	1.1001046918
H	1.0	-3.9221399462	-2.1794999191	1.1002359239
H	1.0	3.9221260801	-2.1795059766	1.1001477984
H	1.0	-3.9526444948	1.2999673338	2.6406449758
H	1.0	3.9523494293	1.2997817761	2.6403461946
H	1.0	-3.9526348367	-1.3000067468	2.6406251314
H	1.0	3.9523446805	-1.2997247072	2.6403718282
H	1.0	-2.4802825065	1.3084773708	1.6566744757
H	1.0	2.4801775206	1.3084540701	1.6561038778
H	1.0	-2.4802741138	-1.3084922029	1.6566520474
H	1.0	2.4801698959	-1.3084071668	1.6561345359

Parent pentamethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at TDDFT-B3LYP-PCM/6-31G(d) excited state optimized structure (S1)

E(S0) = -1153.051169*
E(S1) = -1152.978818

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0000064308	0.0000204589	-1.0637873638
H	1.0	-0.0000594544	0.0000189792	-2.1546520768
C	6.0	-1.2377552881	0.0000278495	-0.4078216402
C	6.0	1.2378082981	0.0000119981	-0.4079728280
H	1.0	-1.2267198072	0.0000265762	0.6782200849
H	1.0	1.2268085181	0.0000156605	0.6780655325
C	6.0	-2.4675740674	0.0000355956	-1.0976805972
C	6.0	2.4676131854	-0.0000063101	-1.0979017436
H	1.0	-2.4027285356	0.0000447733	-2.1834342684
H	1.0	2.4028697960	-0.0000149965	-2.1836848977
C	6.0	-3.7431038807	0.0000286264	-0.5440011387
C	6.0	3.7430954998	-0.0000142524	-0.5441533812
N	7.0	-4.8775191499	0.0000527239	-1.3344768287
N	7.0	4.8775579049	-0.0000544273	-1.3345236920
C	6.0	-4.8532725147	0.0001101292	-2.7908262663
C	6.0	4.8536201982	-0.0001128120	-2.7908692005
H	1.0	-5.8722674350	0.0002305978	-3.1737275019
H	1.0	5.8727178815	-0.0002653406	-3.1735409456
H	1.0	-4.3371000328	0.8923141053	-3.1614657370
H	1.0	4.3379076532	0.8921990666	-3.1618553846
H	1.0	-4.3372724061	-0.8921601728	-3.1615462973
H	1.0	4.3376837160	-0.8923301170	-3.1617711275
C	6.0	-6.0347640839	0.0000107893	-0.5658400999
C	6.0	6.0347646317	-0.0000273064	-0.5658410457
C	6.0	-7.3748536600	0.0000012366	-0.9800275447
C	6.0	7.3747754245	-0.0000357184	-0.9801308035
H	1.0	-7.6536447829	0.0000225951	-2.0281073012
H	1.0	7.6534332314	-0.0000602679	-2.0282613126
C	6.0	-8.3544374995	-0.0000428088	0.0132191394
C	6.0	8.3544340602	-0.0000047666	0.0130260497
H	1.0	-9.4012857132	-0.0000516511	-0.2768284592
H	1.0	9.4012228220	-0.0000102461	-0.2771449741
C	6.0	-8.0138059148	-0.0000775606	1.3750071424
C	6.0	8.0138187403	0.0000346108	1.3748086783
H	1.0	-8.7976701281	-0.0001116817	2.1267419042
H	1.0	8.7976929924	0.0000580217	2.1265283811
C	6.0	-6.6673095404	-0.0000703281	1.7719962309
C	6.0	6.6673396407	0.0000461125	1.7718794042
H	1.0	-6.4095753635	-0.0000993993	2.8278682905
H	1.0	6.4098663316	0.0000788451	2.8278389318
C	6.0	-5.6801726510	-0.0000275238	0.7991042138
C	6.0	5.6801274027	0.0000165814	0.7990788248

C	6.0	-4.1668604253	-0.0000132601	0.9286047773
C	6.0	4.1667805121	0.0000237115	0.9285370480
C	6.0	-3.6877014164	1.2758495511	1.6702689549
C	6.0	3.6874687622	1.2758179686	1.6702806922
C	6.0	-3.6876725834	-1.2758997955	1.6702078171
C	6.0	3.6874629256	-1.2757303726	1.6703478644
H	1.0	-4.0228468803	2.1798573470	1.1519652136
H	1.0	4.0226931579	2.1799906036	1.1523473212
H	1.0	-4.0228017689	-2.1798902768	1.1518632333
H	1.0	4.0226813622	-2.1799313974	1.1524605415
H	1.0	-4.1006382485	1.2880680891	2.6848625076
H	1.0	4.1001222748	1.2877808388	2.6849950803
H	1.0	-4.1006054228	-1.2881736197	2.6848022469
H	1.0	4.1001188488	-1.2876428860	2.6850618716
H	1.0	-2.5973157136	1.3080034261	1.7481333745
H	1.0	2.5970670214	1.3079395817	1.7478506745
H	1.0	-2.5972860597	-1.3080353466	1.7480667164
H	1.0	2.5970612036	-1.3078424040	1.7479218434

Conformationally restrained pentamethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at B3LYP-PCM/6-31G(d) ground state optimized structure (S0)

E(S0) = -1458.455336
E(S1) = -1458.381840*

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0084592318	-0.0735953366	-1.2750030347
C	6.0	-1.2309211688	-0.0314351507	-0.6264955978
C	6.0	1.2136833410	-0.0359358058	-0.5702298260
H	1.0	-1.2146573541	-0.0111144271	0.4582388048
H	1.0	1.1668413111	0.0145488586	0.5130170549
C	6.0	-2.4577156391	-0.0099901840	-1.3039325188
C	6.0	2.4526001867	-0.0326118597	-1.2263042975
C	6.0	-3.6927007969	0.0224394277	-0.6403351511
C	6.0	3.6926978567	0.0143334967	-0.5844191711
N	7.0	-4.8621570978	0.0640186861	-1.3279187227
N	7.0	4.8502286557	0.0678623437	-1.2937034492
C	6.0	-5.9795269358	0.0450439094	-0.4712274671
C	6.0	5.9810576253	0.0474773298	-0.4553272218
C	6.0	-7.3309183308	0.0520837297	-0.8090779030
C	6.0	7.3267393725	0.0610410621	-0.8143655933
H	1.0	-7.6665932836	0.0656009323	-1.8406460376
H	1.0	7.6453710470	0.0829505827	-1.8512517064
C	6.0	-8.2513418929	0.0338690428	0.2461424540
C	6.0	8.2640807574	0.0377278338	0.2261054521
H	1.0	-9.3141387120	0.0382082027	0.0208899049
H	1.0	9.3231606746	0.0460928094	-0.0157994070
C	6.0	-7.8239886419	0.0074098425	1.5779945328
C	6.0	7.8583407903	0.0013576942	1.5644136663
H	1.0	-8.5575613023	-0.0065790259	2.3789247391
H	1.0	8.6046835031	-0.0164282416	2.3533871721
C	6.0	-6.4552393163	-0.0043270200	1.8901251827
C	6.0	6.4946978683	-0.0156216461	1.8981993843
H	1.0	-6.1322363216	-0.0276888162	2.9276809338
H	1.0	6.1880124546	-0.0464332110	2.9404850808
C	6.0	-5.5322996080	0.0121390429	0.8525886003
C	6.0	5.5551337371	0.0044511390	0.8759997081
C	6.0	-4.0099052604	0.0007030535	0.8695237341
C	6.0	4.0330011833	-0.0089508148	0.9180517699
C	6.0	-3.4778229679	1.2657208533	1.5889339295
C	6.0	3.5071877054	1.2546180078	1.6444837336
C	6.0	-3.4979783398	-1.2929070403	1.5501167810
C	6.0	3.5229722921	-1.3012573922	1.6007340775
H	1.0	-3.8318416324	2.1759813312	1.0944605774
H	1.0	3.8523402821	2.1663415231	1.1465186907
H	1.0	-3.8644233500	-2.1824729458	1.0278373290
H	1.0	3.8877255508	-2.1918002996	1.0789892730
H	1.0	-3.8410752816	1.2748854295	2.6221616442

H	1.0	3.8818118520	1.2640766349	2.6736293521
H	1.0	-3.8632201193	-1.3278421121	2.5820303042
H	1.0	3.8879359169	-1.3357361555	2.6327823125
H	1.0	-2.3851458810	1.2915524655	1.6149841365
H	1.0	2.4145970743	1.2757535450	1.6823543967
H	1.0	-2.4059864527	-1.3353110582	1.5770375548
H	1.0	2.4305607587	-1.3405330374	1.6263718857
C	6.0	-4.9660338057	0.1202122127	-2.7896993008
C	6.0	4.9248529042	0.1367118639	-2.7572259254
C	6.0	0.0615581425	-0.1140296778	-2.7895431296
C	6.0	2.4301875880	-0.0681923673	-2.7540782171
C	6.0	-2.4511884657	-0.0186887278	-2.8350970127
C	6.0	-3.6881181551	0.7061497509	-3.3813508652
C	6.0	-1.1520427341	0.5890281078	-3.3881885879
C	6.0	3.6224342636	0.6898914971	-3.3295705741
O	8.0	1.2446103482	0.5311435533	-3.2664248135
H	1.0	5.1394340519	-0.8666313835	-3.1460738453
H	1.0	5.7647233895	0.7845276276	-3.0217670055
H	1.0	3.6388400985	0.5995040297	-4.4196718527
H	1.0	3.5215998848	1.7519295973	-3.0781434588
H	1.0	2.4710614402	-1.1189246237	-3.0920957879
H	1.0	0.0754322176	-1.1644450706	-3.1307830770
H	1.0	-1.1308157078	0.5003703408	-4.4800557498
H	1.0	-1.0998106613	1.6564109570	-3.1369923393
H	1.0	-2.5013003842	-1.0667324550	-3.1715265604
H	1.0	-3.7322343002	0.6187545374	-4.4719613483
H	1.0	-3.6287957648	1.7744205854	-3.1376442718
H	1.0	-5.1534834565	-0.8923571584	-3.1682880955
H	1.0	-5.8320677155	0.7386665137	-3.0407324795

Conformationally restrained pentamethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at TDDFT-B3LYP-PCM/6-31G(d) excited state optimized structure (S1)

E(S0) = -1458.452623*
E(S1) = -1458.382597

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0081819881	-0.0145058967	-1.2157979673
C	6.0	-1.2406223584	0.0027524542	-0.5743874880
C	6.0	1.2257423404	0.0175268663	-0.5151223925
H	1.0	-1.2347621361	0.0134315313	0.5100217677
H	1.0	1.1883540900	0.0665734824	0.5678598978
C	6.0	-2.4732465529	0.0164905124	-1.2675684236
C	6.0	2.4665800447	0.0101197357	-1.1863119680
C	6.0	-3.7174911155	0.0304347844	-0.6244817832
C	6.0	3.7185066510	0.0285787437	-0.5654955080
N	7.0	-4.8946664225	0.0479081925	-1.3432486799
N	7.0	4.8811185548	0.0620920324	-1.3067886467
C	6.0	-6.0079338727	0.0190205500	-0.5175314761
C	6.0	6.0088634097	0.0239505315	-0.5003645406
C	6.0	-7.3631589913	0.0031486667	-0.8743707493
C	6.0	7.3576330913	0.0169271722	-0.8798723575
H	1.0	-7.6822291327	0.0002519527	-1.9111246783
H	1.0	7.6593412710	0.0322078885	-1.9217917238
C	6.0	-8.2954776060	-0.0168348937	0.1640497671
C	6.0	8.3071082888	-0.0197849946	0.1428075828
H	1.0	-9.3550117000	-0.0294743521	-0.0759192941
H	1.0	9.3625855152	-0.0274169652	-0.1143190659
C	6.0	-7.8894661491	-0.0237899201	1.5071353292
C	6.0	7.9234636422	-0.0499718087	1.4921527617
H	1.0	-8.6371531050	-0.0396387273	2.2947713186
H	1.0	8.6840830308	-0.0785659456	2.2669353651
C	6.0	-6.5250887587	-0.0138614831	1.8429787530
C	6.0	6.5650030984	-0.0465874158	1.8507586089
H	1.0	-6.2210245652	-0.0224679565	2.8864271409
H	1.0	6.2778172852	-0.0723729719	2.8986763838
C	6.0	-5.5840399585	0.0050141136	0.8249861596
C	6.0	5.6072095662	-0.0124523621	0.8491643439
C	6.0	-4.0634725588	0.0138765670	0.8733247977
C	6.0	4.0876885712	-0.0004647716	0.9237606404
C	6.0	-3.5596532307	1.2861889222	1.6053671067
C	6.0	3.5973220715	1.2692031179	1.6701092296
C	6.0	-3.5501488156	-1.2681904644	1.5811993730
C	6.0	3.5700125855	-1.2824712930	1.6263824807
H	1.0	-3.9219363159	2.1921281642	1.1091031319
H	1.0	3.9547832259	2.1775879122	1.1749339374
H	1.0	-3.9011276256	-2.1674581204	1.0650999357
H	1.0	3.9154258210	-2.1815713915	1.1063508225
H	1.0	-3.9323377604	1.2871657495	2.6356060668

H	1.0	3.9827984153	1.2626658882	2.6955706093
H	1.0	-3.9285394808	-1.2930842214	2.6089783237
H	1.0	3.9471205132	-1.3139447971	2.6544246069
H	1.0	-2.4676324699	1.3263744780	1.6405585610
H	1.0	2.5057016894	1.3100434866	1.7189356112
H	1.0	-2.4582225869	-1.2992477335	1.6224153961
H	1.0	2.4774931902	-1.3052532140	1.6650354125
C	6.0	-4.9615193999	0.0684932190	-2.8048755923
C	6.0	4.9203817962	0.1133682796	-2.7698158163
C	6.0	0.0614728268	-0.0539707616	-2.7288819469
C	6.0	2.4251006162	-0.0266116726	-2.7120587480
C	6.0	-2.4456647989	0.0090660058	-2.7960195617
C	6.0	-3.6916224230	0.6935259758	-3.3721327593
C	6.0	-1.1522432821	0.6405272095	-3.3338405889
C	6.0	3.6217935142	0.7045160541	-3.3121260798
O	8.0	1.2426541786	0.5849042915	-3.2118558906
H	1.0	5.0812284370	-0.9024088362	-3.1558865967
H	1.0	5.7771111442	0.7235932189	-3.0678312952
H	1.0	3.6099699559	0.6132370597	-4.4022569610
H	1.0	3.5543063345	1.7687116726	-3.0591021872
H	1.0	2.4443163882	-1.0825275105	-3.0402776904
H	1.0	0.0731228125	-1.1095712729	-3.0593976307
H	1.0	-1.1193672076	0.5562314728	-4.4257002762
H	1.0	-1.1169408484	1.7073057779	-3.0776495020
H	1.0	-2.4614224207	-1.0441234943	-3.1240922260
H	1.0	-3.7075410509	0.5966454749	-4.4628293631
H	1.0	-3.6714395736	1.7648355603	-3.1354298726
H	1.0	-5.0892467519	-0.9602723274	-3.1689112650
H	1.0	-5.8465764089	0.6397097468	-3.0981698800

Parent heptamethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at B3LYP-PCM/6-31G(d) ground state optimized structure (S0)

E(S0) = -1230.195344
E(S1) = -1230.127389*

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1202319192	-0.0865120271	-0.5365065399
C	6.0	-1.1214084499	-0.0945812173	-1.1777963159
C	6.0	1.3523865762	-0.0780320974	-1.1957749303
C	6.0	-2.3337854712	-0.1035412122	-0.4893331669
C	6.0	2.5747331635	-0.0692996081	-0.5251584032
H	1.0	-2.2835612742	-0.1043947446	0.5963982325
H	1.0	2.5397619200	-0.0689223295	0.5612222669
C	6.0	-3.5841502047	-0.1109892223	-1.1229103965
C	6.0	3.8157592789	-0.0608082160	-1.1767154328
H	1.0	-3.5719057804	-0.1084603646	-2.2096391114
H	1.0	3.7884194410	-0.0624525121	-2.2631270226
C	6.0	-4.8313092567	-0.1216383812	-0.5025584493
C	6.0	5.0718195146	-0.0510773510	-0.5745217571
N	7.0	-5.9859593490	-0.1266289084	-1.2213895797
N	7.0	6.2160278429	-0.0389730356	-1.3098482009
C	6.0	-6.0460381578	-0.1196407877	-2.6794823704
C	6.0	6.2547757577	-0.0313612115	-2.7687077119
H	1.0	-7.0871423837	-0.1184763610	-2.9962386791
H	1.0	7.2898434871	0.0177936860	-3.1012688611
H	1.0	-5.5551474379	-1.0100627549	-3.0846708676
H	1.0	5.7977813286	-0.9428450287	-3.1669614820
H	1.0	-5.5565190349	0.7755705743	-3.0754646042
H	1.0	5.7202513640	0.8409667688	-3.1569883961
C	6.0	-7.1212805762	-0.1406377858	-0.3821319358
C	6.0	7.3633683558	-0.0380691395	-0.4869891187
C	6.0	-8.4699335200	-0.1505114825	-0.7325796138
C	6.0	8.7070864019	-0.0323485612	-0.8560368995
H	1.0	-8.8002306231	-0.1483880026	-1.7657461137
H	1.0	9.0228198466	-0.0294756366	-1.8937356231
C	6.0	-9.4045516313	-0.1640612268	0.3100070479
C	6.0	9.6562060954	-0.0317971635	0.1735603408
H	1.0	-10.4637408834	-0.1720920381	0.0683852831
H	1.0	10.7119975814	-0.0275604416	-0.0824243616
C	6.0	-8.9976978005	-0.1675193106	1.6481739903
C	6.0	9.2680829334	-0.0371493002	1.5173519994
H	1.0	-9.7420416427	-0.1781963541	2.4391227487
H	1.0	10.0233968801	-0.0366254589	2.2979086893
C	6.0	-7.6334156193	-0.1573574233	1.9761896791
C	6.0	7.9085596174	-0.0439326286	1.8641261611
H	1.0	-7.3217033262	-0.1601382856	3.0174814149
H	1.0	7.6110121079	-0.0488348092	2.9095221255
C	6.0	-6.6968133591	-0.1439494664	0.9508697944

C	6.0	6.9578748621	-0.0448670452	0.8519008856
C	6.0	-5.1768353091	-0.1310804453	0.9965930076
C	6.0	5.4387291675	-0.0532212960	0.9193522481
C	6.0	-4.6474677651	-1.4072089803	1.6964705019
C	6.0	4.9374473821	-1.3355975829	1.6284223509
C	6.0	-4.6693699420	1.1481258083	1.7071795879
C	6.0	4.9233080749	1.2199161289	1.6351177916
H	1.0	-4.9952645285	-2.3096670876	1.1836286278
H	1.0	5.2910563703	-2.2338248381	1.1121657320
H	1.0	-5.0331762552	2.0486771029	1.2021621316
H	1.0	5.2675508484	2.1246899304	1.1239705371
H	1.0	-5.0151740965	-1.4362875917	2.7277337228
H	1.0	5.3194114685	-1.3578800770	2.6546394068
H	1.0	-5.0369728463	1.1622613003	2.7388140906
H	1.0	5.3044468395	1.2406415218	2.6616896110
H	1.0	-3.5545389873	-1.4280869038	1.7261668572
H	1.0	3.8454421744	-1.3719462736	1.6729955036
H	1.0	-3.5769705442	1.1874952719	1.7365930358
H	1.0	3.8309164875	1.2444258350	1.6791199030
H	1.0	0.1277944498	-0.0867394768	0.5546806673
H	1.0	-1.1416051403	-0.0939581799	-2.2674902444
H	1.0	1.3571966679	-0.0780540440	-2.2856701444

Parent heptamethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at TDDFT-B3LYP-PCM/6-31G(d) excited state optimized structure (S1)

E(S0) = -1230.193281*
E(S1) = -1230.127874

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1217301350	-0.0908646696	-0.3698829340
C	6.0	-1.1210636339	-0.0977134702	-1.0195107242
C	6.0	1.3546769165	-0.0826714740	-1.0380597416
C	6.0	-2.3522596810	-0.1063063035	-0.3567509436
C	6.0	2.5955663799	-0.0735405674	-0.3936807809
H	1.0	-2.3323640260	-0.1084398330	0.7294004470
H	1.0	2.5910703764	-0.0725384717	0.6926191210
C	6.0	-3.5873020948	-0.1118514660	-1.0343727723
C	6.0	3.8204255516	-0.0644592533	-1.0895123611
H	1.0	-3.5343089409	-0.1076377792	-2.1206963279
H	1.0	3.7511113036	-0.0666148083	-2.1749464395
C	6.0	-4.8573352303	-0.1223653947	-0.4666206470
C	6.0	5.0985408228	-0.0530597482	-0.5403015579
N	7.0	-5.9960111820	-0.1257825612	-1.2410410252
N	7.0	6.2263372417	-0.0400649023	-1.3304104208
C	6.0	-5.9905569409	-0.1168928897	-2.6981217509
C	6.0	6.2002885510	-0.0320058109	-2.7872423300
H	1.0	-7.0147626137	-0.1173532214	-3.0666843200
H	1.0	7.2181380629	0.0154098746	-3.1702205471
H	1.0	-5.4773443076	-1.0053380443	-3.0813608866
H	1.0	5.7221534487	-0.9424509362	-3.1647063346
H	1.0	-5.4825636585	0.7793106941	-3.0699353658
H	1.0	5.6472192706	0.8404951442	-3.1502508399
C	6.0	-7.1492565621	-0.1390484857	-0.4573088073
C	6.0	7.3903893612	-0.0371577191	-0.5626642210
C	6.0	-8.4912057378	-0.1473381738	-0.8576321196
C	6.0	8.7267774592	-0.0300261466	-0.9810818913
H	1.0	-8.7811953747	-0.1440237575	-1.9027148728
H	1.0	9.0026731247	-0.0277598571	-2.0300255073
C	6.0	-9.4615740186	-0.1605771640	0.1465250092
C	6.0	9.7107429680	-0.0274886347	0.0098913069
H	1.0	-10.5112079563	-0.1673018350	-0.1334131361
H	1.0	10.7564603190	-0.0220726717	-0.2842281953
C	6.0	-9.1068061292	-0.1654733145	1.5031738100
C	6.0	9.3743860508	-0.0322739278	1.3712846003
H	1.0	-9.8822419064	-0.1758317780	2.2635872867
H	1.0	10.1600150644	-0.0301257143	2.1212245644
C	6.0	-7.7561071685	-0.1570583048	1.8851611111
C	6.0	8.0290836712	-0.0405600690	1.7714342800
H	1.0	-7.4864461194	-0.1610223520	2.9380788200
H	1.0	7.7737656491	-0.0448398479	2.8279690266
C	6.0	-6.7796406164	-0.1438797267	0.9006600740

C	6.0	7.0394135178	-0.0434775594	0.8002671445
C	6.0	-5.2644806250	-0.1327919706	1.0119272492
C	6.0	5.5259112333	-0.0529344927	0.9324234017
C	6.0	-4.7665086152	-1.4087718917	1.7394914622
C	6.0	5.0560187338	-1.3327596141	1.6717981511
C	6.0	-4.7860766811	1.1435466214	1.7520289932
C	6.0	5.0404060203	1.2196899749	1.6745255994
H	1.0	-5.1010536936	-2.3123391340	1.2200083771
H	1.0	5.3949364942	-2.2337262525	1.1506567126
H	1.0	-5.1329051382	2.0469378038	1.2403379121
H	1.0	5.3699771251	2.1257957279	1.1562965752
H	1.0	-5.1675546673	-1.4300777653	2.7586656020
H	1.0	5.4723034957	-1.3449723130	2.6850012858
H	1.0	-5.1888787241	1.1498241291	2.7707287916
H	1.0	5.4549360502	1.2338089150	2.6884199492
H	1.0	-3.6751093029	-1.4332654582	1.8042612807
H	1.0	3.9661444749	-1.3717729713	1.7532279665
H	1.0	-3.6952329689	1.1830188055	1.8188879576
H	1.0	3.9499883623	1.2462280891	1.7539816013
H	1.0	0.1295796104	-0.0915186211	0.7204897277
H	1.0	-1.1265994953	-0.0961726504	-2.1103439068
H	1.0	1.3445719736	-0.0828717796	-2.1288638490

Conformationally restrained heptamethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at B3LYP-PCM/6-31G(d) ground state optimized structure (S0)

E(S0) = -1612.777156
E(S1) = -1612.712866*

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1205005513	-0.1995659869	-0.5687812589
C	6.0	-1.1049228187	-0.2125615322	-1.2431553690
C	6.0	1.3370010370	-0.1987378847	-1.2594547020
C	6.0	-2.3293852387	-0.1721756409	-0.5718260738
C	6.0	2.5699697221	-0.1402004504	-0.6052631709
H	1.0	-2.2931345181	-0.1724639693	0.5125885952
H	1.0	2.5478977102	-0.1343567376	0.4796022340
C	6.0	-3.5717973122	-0.1272452182	-1.2251282257
C	6.0	3.8029548187	-0.0854673495	-1.2758964153
C	6.0	-4.7912747412	-0.0966539272	-0.5384402866
C	6.0	5.0315340853	-0.0324403041	-0.6071353811
N	7.0	-5.9765058345	-0.0285650950	-1.2021709175
N	7.0	6.2065384180	0.0383455310	-1.2889299840
C	6.0	-7.0750402981	-0.0566903584	-0.3237854649
C	6.0	7.3176286219	0.0404808526	-0.4262413086
C	6.0	-8.4335836238	-0.0283856815	-0.6319849261
C	6.0	8.6711514173	0.0790819053	-0.7547940186
H	1.0	-8.7914081879	0.0135834886	-1.6554318329
H	1.0	9.0131145594	0.1043811996	-1.7841393322
C	6.0	-9.3321634557	-0.0626203108	0.4416850655
C	6.0	9.5855061503	0.0776080453	0.3060027416
H	1.0	-10.3993216795	-0.0427535019	0.2386082064
H	1.0	10.6493108753	0.1064009568	0.0870209410
C	6.0	-8.8779192190	-0.1252679492	1.7633018196
C	6.0	9.1511213426	0.0366352432	1.6351276846
H	1.0	-9.5946614722	-0.1515337546	2.5790538931
H	1.0	9.8798052844	0.0362468837	2.4406686208
C	6.0	-7.5029545178	-0.1570943750	2.0458583759
C	6.0	7.7808489807	-0.0074914477	1.9382893514
H	1.0	-7.1586143485	-0.2081878760	3.0756532182
H	1.0	7.4518773631	-0.0425827785	2.9737175830
C	6.0	-6.6015596016	-0.1246300435	0.9901963834
C	6.0	6.8639950783	-0.0079302297	0.8954756291
C	6.0	-5.0789563082	-0.1480318058	0.9765903325
C	6.0	5.3419945744	-0.0550302256	0.9043740169
C	6.0	-4.5635075191	-1.4579325085	1.6220438318
C	6.0	4.8575100479	-1.3635384571	1.5766097711
C	6.0	-4.5244374427	1.0982602123	1.7119126505
C	6.0	4.7764929810	1.1925382304	1.6285273941
H	1.0	-4.9450594405	-2.3346316641	1.0888700790
H	1.0	5.2461050668	-2.2418044507	1.0511624701
H	1.0	-4.8863092561	2.0207383330	1.2464643891

H	1.0	5.1093656608	2.1139044560	1.1398508572
H	1.0	-4.9105520182	-1.5110508927	2.6595327170
H	1.0	5.2195069351	-1.3959508838	2.6098501969
H	1.0	-4.8631613364	1.0858402405	2.7535289687
H	1.0	5.1353783674	1.2058393486	2.6633431544
H	1.0	-3.4714955373	-1.5074063795	1.6286603334
H	1.0	3.7666566984	-1.4304912014	1.5990890500
H	1.0	-3.4313069858	1.1195578487	1.7124133190
H	1.0	3.6833315393	1.1910868720	1.6502787857
H	1.0	0.1272004414	-0.1639595224	0.5205120074
C	6.0	6.3152881642	0.1050839717	-2.7490965989
C	6.0	-6.1070872924	0.0610486005	-2.6594230889
C	6.0	-3.5942030083	-0.1059258694	-2.7559555166
C	6.0	-1.0807601162	-0.2305137467	-2.7618387896
C	6.0	1.2911027223	-0.2218841780	-2.7776128316
C	6.0	3.8028597999	-0.0794907563	-2.8071495693
C	6.0	-4.8330979983	0.6441652135	-3.2630595575
C	6.0	-2.2985509250	0.4968349180	-3.3230673147
C	6.0	5.0290423283	0.6717700543	-3.3420629198
C	6.0	2.4953746891	0.5107400869	-3.3599376671
O	8.0	0.0994927962	0.3997279054	-3.2629747923
H	1.0	7.1709043088	0.7406171578	-2.9937506948
H	1.0	6.5223263277	-0.9012954589	-3.1346822521
H	1.0	-6.3146455376	-0.9402814539	-3.0576219333
H	1.0	-6.9697132357	0.6955755200	-2.8812236418
H	1.0	-4.7557183947	1.7059900043	-2.9970040297
H	1.0	4.9488264426	1.7366574212	-3.0895118139
H	1.0	5.0793463263	0.5946296086	-4.4332180647
H	1.0	-4.8991369053	0.5818580287	-4.3542671835
H	1.0	-2.2999382899	0.4286334155	-4.4167213907
H	1.0	-2.2289142236	1.5588078393	-3.0533679481
H	1.0	2.4820003413	0.4358859686	-4.4530716250
H	1.0	2.4222002983	1.5738392767	-3.0957461803
H	1.0	3.8717560779	-1.1232746615	-3.1535526228
H	1.0	1.3047137863	-1.2705527102	-3.1262621824
H	1.0	-1.0934234402	-1.2781046323	-3.1138239330
H	1.0	-3.6629733388	-1.1465037569	-3.1118936875

Conformationally restrained heptamethine indocyanine: ORMAS-PT2-PCM/6-31G(d) energies at TDDFT-B3LYP-PCM/6-31G(d) excited state optimized structure (S1)

E(S0) = -1612.775352*
E(S1) = -1612.713153

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1209720074	-0.1053162816	-0.4962603579
C	6.0	-1.1097520742	-0.1284349329	-1.1734659763
C	6.0	1.3421602779	-0.1120062312	-1.1906662419
C	6.0	-2.3475766713	-0.1114769886	-0.5153389963
C	6.0	2.5890792133	-0.0785599189	-0.5502438604
H	1.0	-2.3260489801	-0.1066040013	0.5691049895
H	1.0	2.5821866864	-0.0749509747	0.5344421295
C	6.0	-3.5886943865	-0.0948067795	-1.1889376257
C	6.0	3.8200860535	-0.0435025940	-1.2414742074
C	6.0	-4.8228266839	-0.0883646313	-0.5265006884
C	6.0	5.0635667573	-0.0199957184	-0.5970544450
N	7.0	-6.0076932788	-0.0626656615	-1.2229707520
N	7.0	6.2377602382	0.0224885805	-1.3105887481
C	6.0	-7.1112246037	-0.1057760537	-0.3769938724
C	6.0	7.3539772691	-0.0034924429	-0.4806671612
C	6.0	-8.4697268609	-0.1192430200	-0.7127554872
C	6.0	8.7076277588	0.0017004490	-0.8357200935
H	1.0	-8.8057185453	-0.1067087864	-1.7441868215
H	1.0	9.0284530590	0.0169268285	-1.8719179227
C	6.0	-9.3866140231	-0.1577457986	0.3406412335
C	6.0	9.6399454700	-0.0218331988	0.2045718512
H	1.0	-10.4496909864	-0.1695219776	0.1164414625
H	1.0	10.6998230716	-0.0191418150	-0.0344572685
C	6.0	-8.9595183363	-0.1843935796	1.6754851597
C	6.0	9.2323461686	-0.0517179089	1.5455071472
H	1.0	-9.6939847233	-0.2145034511	2.4751208247
H	1.0	9.9785509504	-0.0695573906	2.3345816933
C	6.0	-7.5898970018	-0.1757416629	1.9889843547
C	6.0	7.8674150653	-0.0624969363	1.8783694775
H	1.0	-7.2685367541	-0.1994081698	3.0270912204
H	1.0	7.5608669024	-0.0890311494	2.9208497734
C	6.0	-6.6655781961	-0.1388894875	0.9554801283
C	6.0	6.9281475468	-0.0410667797	0.8580635036
C	6.0	-5.1439204639	-0.1256390003	0.9777743751
C	6.0	5.4070422603	-0.0513222131	0.9023875872
C	6.0	-4.6139851256	-1.4145513439	1.6586002187
C	6.0	4.9069603282	-1.3477643361	1.5915084359
C	6.0	-4.6326561462	1.1396857810	1.7156848975
C	6.0	4.8867474176	1.2065689826	1.6466891890
H	1.0	-4.9706224291	-2.3081445983	1.1364807112
H	1.0	5.2699782448	-2.2361456343	1.0649164600
H	1.0	-5.0099207795	2.0498360886	1.2385789240

H	1.0	5.2400830338	2.1221248936	1.1616666490
H	1.0	-4.9752353561	-1.4546514179	2.6920697588
H	1.0	5.2830380248	-1.3816500260	2.6198738153
H	1.0	-4.9856873171	1.1252098480	2.7527535917
H	1.0	5.2572255617	1.2002931634	2.6777037394
H	1.0	-3.5214187510	-1.4421879829	1.6810832703
H	1.0	3.8153785343	-1.3920406107	1.6291952453
H	1.0	-3.5404391517	1.1860739777	1.7304888347
H	1.0	3.7942502796	1.2345168887	1.6796533189
H	1.0	0.1281021723	-0.0637919614	0.5920352292
C	6.0	6.3110317263	0.0754323893	-2.7715077679
C	6.0	-6.1020757089	-0.0156981601	-2.6828598357
C	6.0	-3.5864171193	-0.0904437813	-2.7181974092
C	6.0	-1.0773931597	-0.1640264968	-2.6900935515
C	6.0	1.2892644237	-0.1470826456	-2.7067159818
C	6.0	3.7962271780	-0.0370859004	-2.7705454687
C	6.0	-4.8380141851	0.6082376292	-3.2645835878
C	6.0	-2.2985375256	0.5371024357	-3.2731525519
C	6.0	5.0292764659	0.6814188996	-3.3332501116
C	6.0	2.4915643356	0.5725567489	-3.3059761115
O	8.0	0.0979796665	0.4660172260	-3.1965421434
H	1.0	7.1829116993	0.6755285466	-3.0466119448
H	1.0	6.4674579631	-0.9413063628	-3.1566558465
H	1.0	-6.2474396192	-1.0362631237	-3.0622319717
H	1.0	-6.9871273543	0.5693638046	-2.9479999154
H	1.0	-4.8066982960	1.6762735107	-3.0145179968
H	1.0	4.9853977621	1.7482140840	-3.0799792533
H	1.0	5.0505696855	0.6020870755	-4.4253056307
H	1.0	-4.8738501546	0.5257332300	-4.3559975698
H	1.0	-2.2830833773	0.4573970942	-4.3658755750
H	1.0	-2.2546932566	1.6028193706	-3.0135128230
H	1.0	2.4616323053	0.4943860969	-4.3984743533
H	1.0	2.4361471170	1.6370957124	-3.0438553606
H	1.0	3.8360161683	-1.0856244147	-3.1104953883
H	1.0	1.3022489553	-1.2030851368	-3.0372258380
H	1.0	-1.0792290095	-1.2203295169	-3.0197868329
H	1.0	-3.6156320930	-1.1401633294	-3.0557196830

Section S7. References

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