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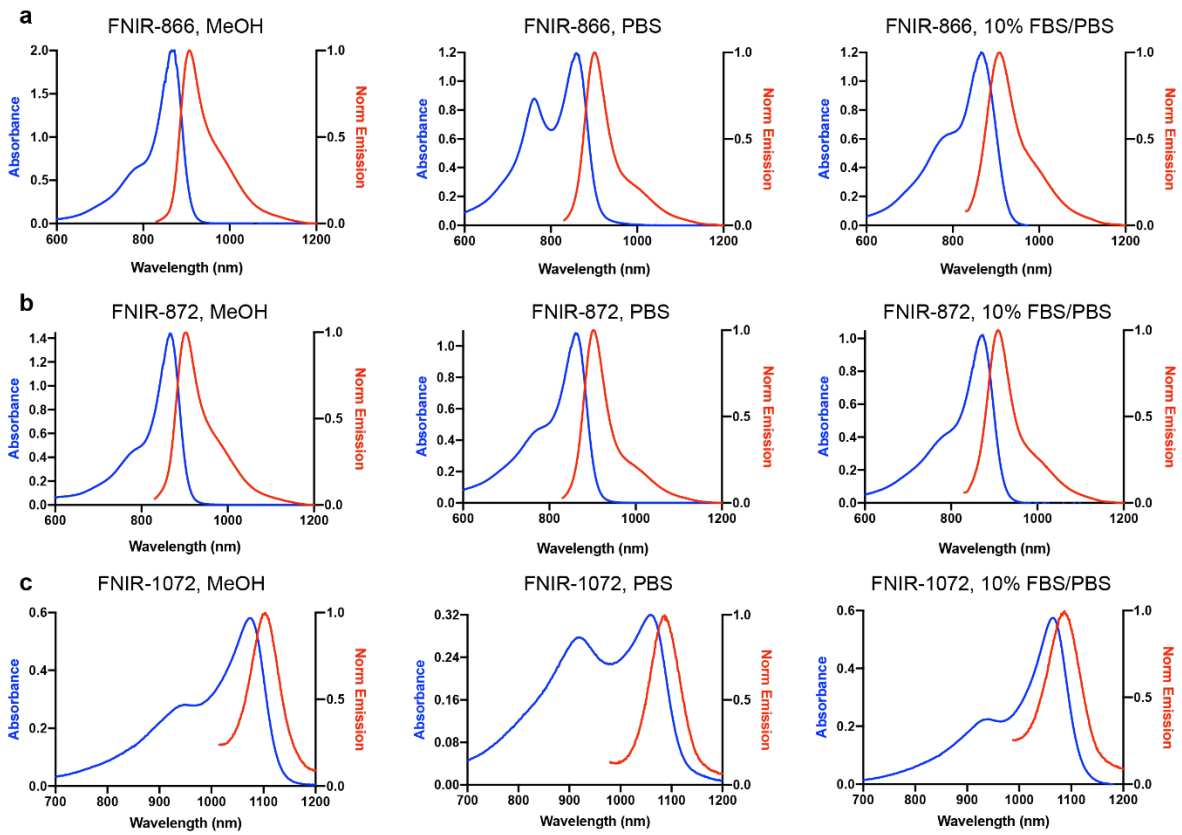
Supplementary information

Targeted multicolor in vivo imaging over 1,000 nm enabled by nonamethine cyanines

In the format provided by the authors and unedited

Supplementary Figures and Tables

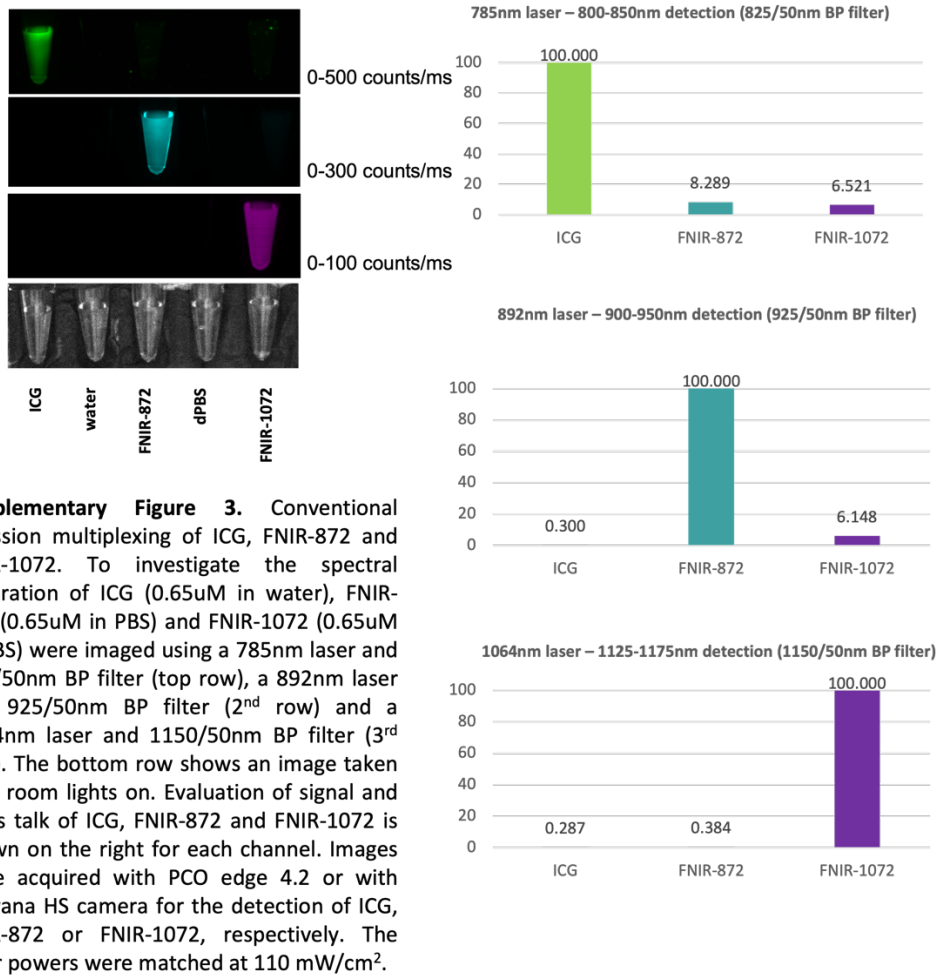


Supplementary Figure 1
Absorbance and emission curves of Cy9 derivatives

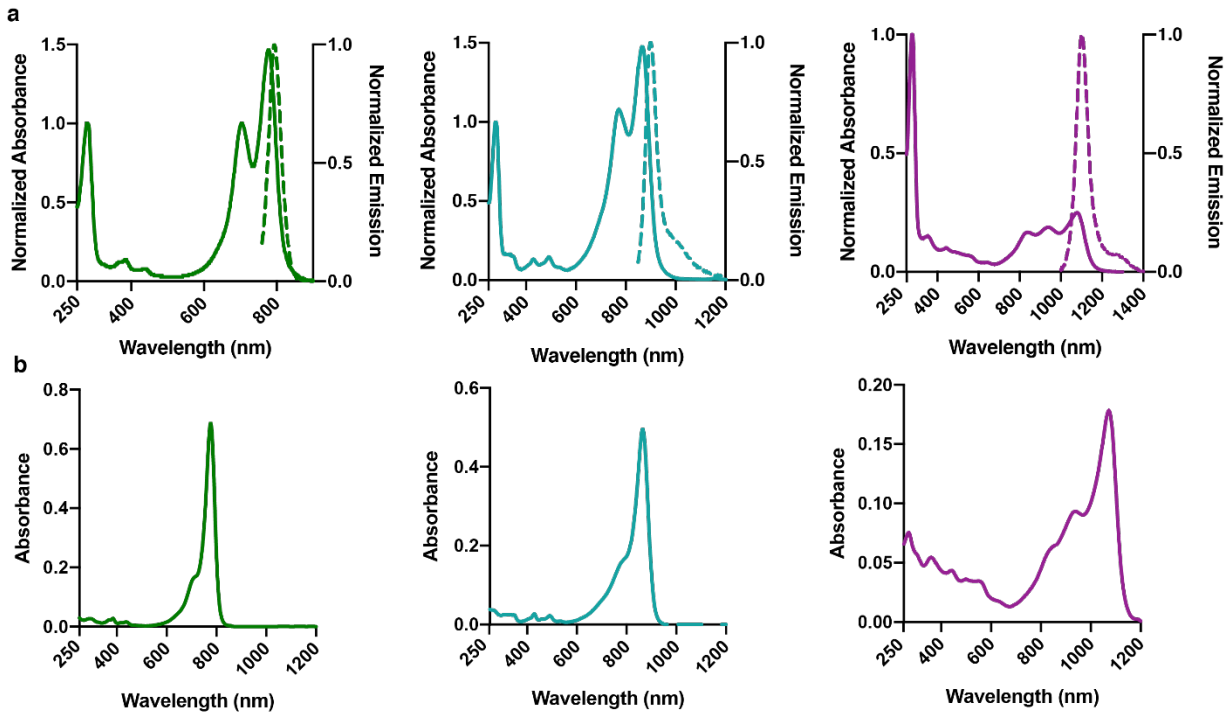
Normalized absorbance and emission curves of 5 μM FNIR-866 **a**, FNIR-872 **b**, and FNIR-1072 **c**, in MeOH, PBS and 10% FBS/PBS (left to right).

Compound	Solvent	λ_{abs} (nm)	λ_{em} (nm)	ε (x 10^5 M^{-1} cm^{-1})	Φ_F (%)
FNIR-866	MeOH	866	896	2.1	3.5
	PBS	860	896	1.9	–
	10% FBS/PBS	868	896	1.9	1.6
FNIR-872	MeOH	869	896	1.9	3.2
	PBS	862	896	1.5	–
	MeOH/PBS	866	–	2.4	–
	10% FBS/PBS	871	900	1.4	1.3
FNIR-1072	MeOH	1072	1103	1.2	0.13
	PBS	1058	1084	0.7	0.056
	MeOH/PBS	1072	–	0.8	
	10% FBS/PBS	1062	1086	1.0	0.10

Supplementary Figure 2
Photophysical properties of Cy9 derivatives

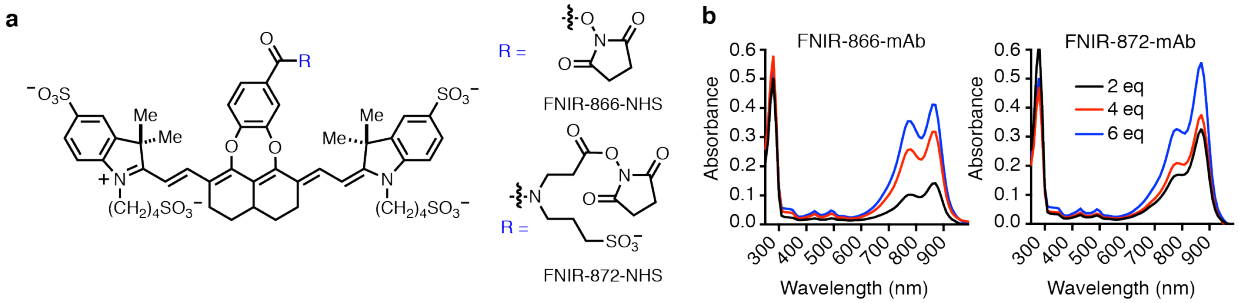


Supplementary Figure 3. Conventional emission multiplexing of ICG, FNIR-872 and FNIR-1072. To investigate the spectral separation of ICG (0.65uM in water), FNIR-872 (0.65uM in PBS) and FNIR-1072 (0.65uM in PBS) were imaged using a 785nm laser and 825/50nm BP filter (top row), a 892nm laser and 925/50nm BP filter (2nd row) and a 1064nm laser and 1150/50nm BP filter (3rd row). The bottom row shows an image taken with room lights on. Evaluation of signal and cross talk of ICG, FNIR-872 and FNIR-1072 is shown on the right for each channel. Images were acquired with PCO edge 4.2 or with NIRvana HS camera for the detection of ICG, FNIR-872 or FNIR-1072, respectively. The laser powers were matched at 110 mW/cm^2.



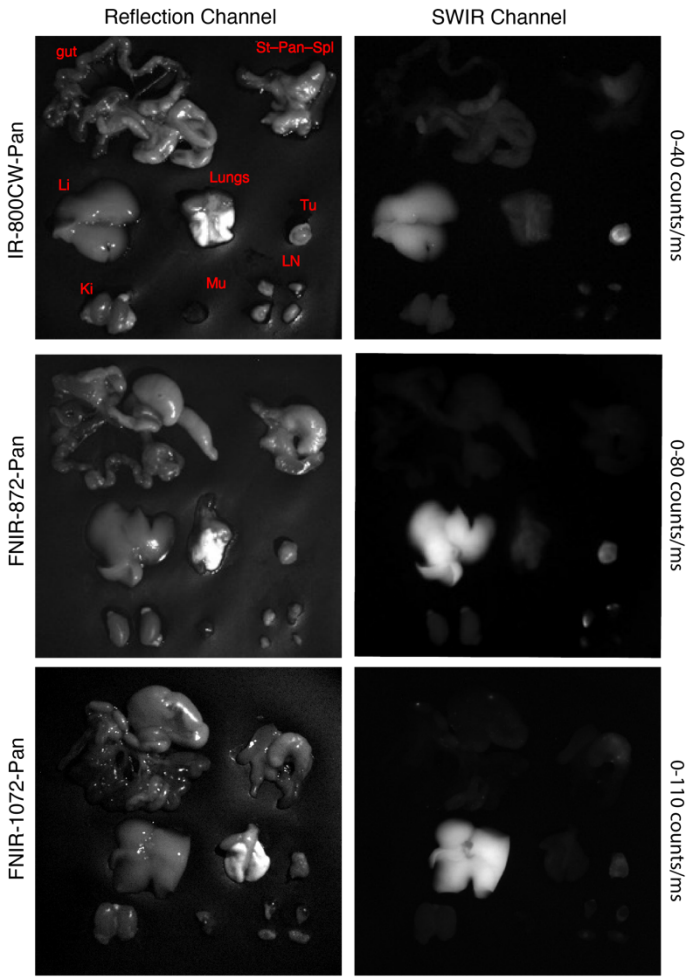
Supplementary Figure 4

a, Normalized absorbance and emission spectra of IR-800CW-Pan (DOL 1.7), FNIR-872-Pan (DOL 1.4) and FNIR-1072-Pan (DOL 1.0) in PBS (50 mM, PBS 7.4). **b**, Full absorbance spectra of IR-800CW, FNIR-872 and FNIR-1072 at a concentration of 2.5 µM in 1/1 (vol/vol) MeOH/PBS. Correction factors ($A_{280}/A_{\lambda max}$) were determined to be 0.04. 0.06 and 0.39 for IR-800CW, FNIR-872 and FNIR-1072, respectively.



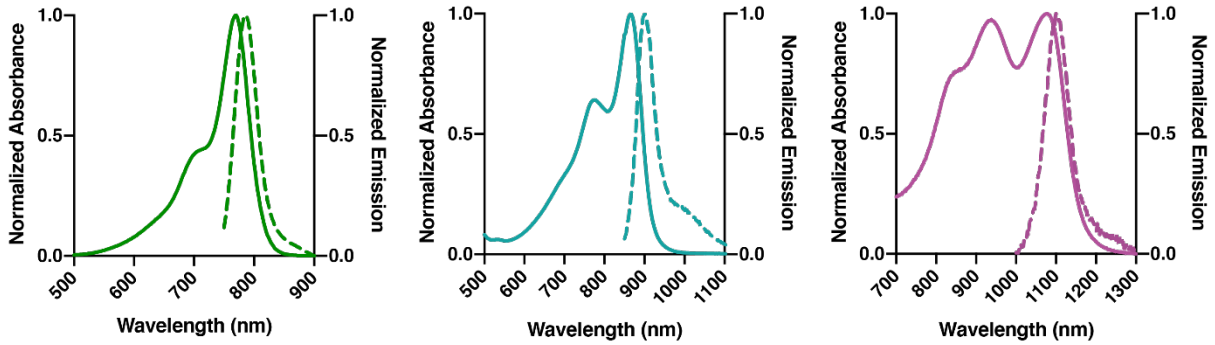
Supplementary Figure 5

a, structures of tetrasulfonated FNIR-866 and pentasulfonated FNIR-872 NHS esters. **b**, absorbance curves (ca. 250 nM mAb concentration) of panitumumab labeled with FNIR-866 or FNIR-872 (2, 4 or 6 eq).

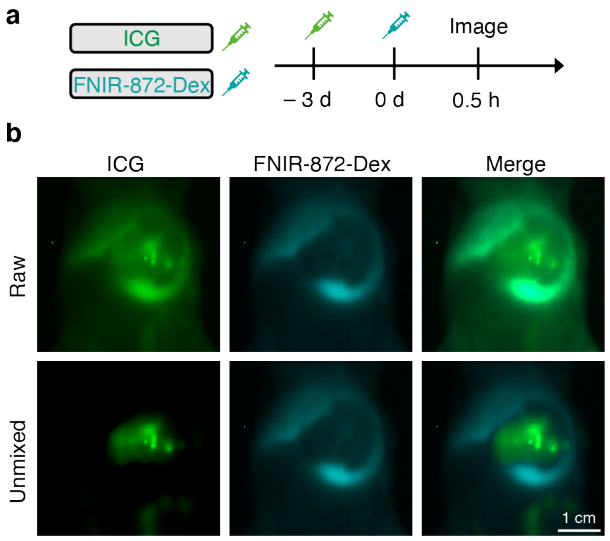


Supplementary Figure 6
ex vivo biodistribution of IR-800CW-Pan, FNIR-872-Pan, and FNIR-1072-Pan

ex vivo images of harvested organs from MDA-MB-468 orthotopic (mammary fat pad) bearing mice 48 h after receiving IR-800CW-Pan (100 µg, DOL 1.9, 1.2 nmol effective dye in 100 µL PBS, i.v.), FNIR-872-Pan (114 µg, DOL 1.0, 0.8 nmol effective dye in 100 µL PBS, i.v.) or FNIR-1072-Pan (112 µg, DOL 1.4, 1.1 nmol effective dye in 100 µL PBS, i.v.). SWIR images of IR-800CW-Pan, FNIR-872-Pan and FNIR-1072 were captured using 785 nm (70 mW/cm^2), 890 nm (70 mW/cm^2) and 968 nm (240 mW/cm^2) acquisition settings, respectively. Anatomy and precise location of the organs was obtained using the reflection channel (1300nm LED, 10 ms). Higher fluorescent signal was depicted at the tumor and at the liver in comparison to other organs.
Images were acquired with Allied Vision G-32 camera using the following filter settings for the detection of IR-800CW, FNIR-872 or FNIR-1072: 1X or 2X 1150 nm long pass filters.

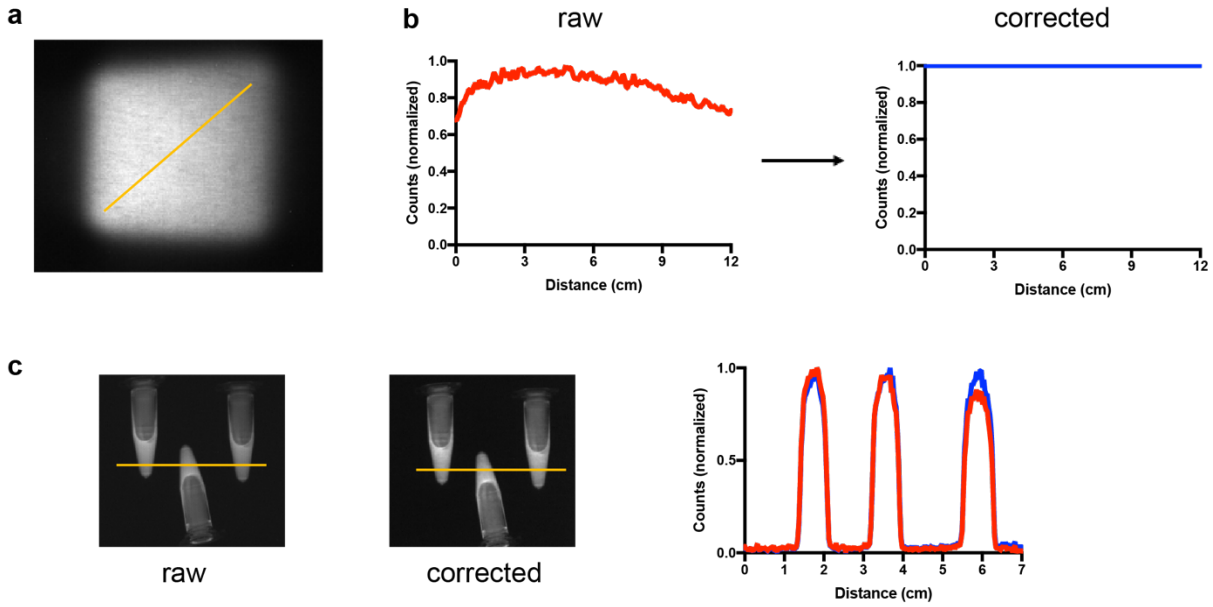


Supplementary Figure 7
Normalized absorbance and emission spectra of FNIR-Tag-Dex, FNIR-872-Dex and FNIR-1072-Dex in PBS (50 mM, PBS 7.4).



Supplementary Figure 8
Spectral unmixing of **Fig 3b** images

a, Dosing scheme for 2-color *in vivo* SWIR imaging of a mouse bearing a Hep3B orthotopic liver tumor. **b**, raw and spectrally unmixed images of Hep3B orthotopic tumor bearing mouse. FNIR-872-Dex signal in the ICG channel can be verified by imaging in the FNIR-872-Dex channel. The healthy surrounding liver tissue in this case is colored blue-green due to the presence of signal in both channels. The ICG channel was spectrally unmixed by subtracting the normalized image of the FNIR-872-Dex channel from the normalized image of the ICG channel. Imaging settings: Images were acquired on a NIRvana 640ST using 3x 1150 long pass filters. The lasers (785 nm for ICG and 890 nm for FNIR-872-Dex) were power matched at 100 mW/cm^2 measured over the tumor for each imaging timepoint. Camera exposure times were 400 ms and 300 ms for the ICG and FNIR-872-Dex channels, respectively. Image scale is 0-50 and 0-150 counts/msec for the 785 and 890 channels, respectively.



Supplementary Figure 9
Flatfield correction

Flatfield correction using reverse side of laser protective material (Thorlabs part # BK5). **a**, Sample normalized flatfield image using 785 nm excitation (100 mW/cm^2) with line drawn representing the line profile in **b**. **b**, normalized plot profile of raw and flatfield corrected image of 785 nm laser projected onto laser protective material. **c**, raw and flatfield corrected image of three microcentrifuge tubes containing IR-780 (1 µM, MeOH) with normalized plot profile of raw and corrected images.

Supplementary Note 1: Computational Chemistry

The GAMESS[1,2] package was employed for all quantum chemistry computations in which 6-31G(d)[3] basis sets were used throughout. The MacMolPlt[4] program was used to illustrate molecular orbitals. Density functional theory (DFT)[5] utilizing the B3LYP[6,7,8] functional was used to optimize ground state (S0) geometries. The time-dependent density functional theory (TDDFT) method[9,10,11,12,13,14,15] 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). Ground state (S0) DFT and excited state

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[1] Schmidt, M. W.; Baldridge, K. K.; Boatz, J. A.; Elbert, S. T.; Gordon, M. S.; Jensen, J. H.; Koseki, S.; Matsunaga, N.; Nguyen, K. A.; Su, S. J.; Windus, T. L.; Dupuis, M.; Montgomery, J. A. The General Atomic and Molecular Electronic Structure System. *J. Comput. Chem.* **1993**, *14*, 1347−1363. See http://www.msg.ameslab.gov/advances/updatepaper.html for a current list of features.

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[3] Hehre, W. J.; Ditchfield, R.; Pople, J. A. Self-Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian-type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1972**, *56*, 2257−2261.

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[6] Becke, A. D. Density-Functional Thermochemistry. III. The Role of Exact Exchange. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

[7] Stephens, P. J.; Devlin, F. J.; Chablowski, C. F.; Frisch, M. J. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields. *J. Phys. Chem.* **1994**, *98*, 11623-11627.

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[14] Chiba, M.; Federov, D. G.; Kitaura, K. in *The Fragment Molecular Orbital Method: Practical Applications to Large Molecular Systems*, edited by D. G. Federov and K. Kitaura (CRC, Boca Raton, 2009), pp. 91–118.

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(S1) TDDFT computations used the Euler-MacLaurin[16] radial and Lebedev[17] angular grids with respective dimensions (96, 302) and (48, 110). The occupation restricted multiple active space (ORMAS)[18,19] method with second-order perturbation theory correction (ORMAS-PT2)[20] was also used to compute vertical excitation (absorbance) energies and deexcitation (emission) energies. ORMAS-PT2 calculations were performed at B3LYP/6-31G(d) ground state (S0; vertical excitation energy) and TDDFT-B3LYP/6-31G(d) excited state (S1; deexcitation energy) optimized geometries. The ORMAS configuration interaction (CI) spaces were constructed and optimized 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*e*, 2*o*) active space)

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

and apply all single and double excitations out of this *base* reference and into a virtual orbital space containing only the remaining commensurate anti-bonding valence π orbitals. HOMO and LUMO refer to the highest occupied molecular orbital and lowest unoccupied molecular orbital, respectively, in a closed-shell wave function. The ORMAS S0 and S1 wave functions were then simultaneously optimized (for all orbitals and CI coefficients) by minimizing the average of the energies of the ground (S0) and excited (S1) singlet states.

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[16] Murray, C. W.; Handy, N. C.; Laming, G. Quadrature Schemes for Integrals of Density Functional Theory. *J. Mol. Phys.* **1993**, *78*, 997-1014.

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[18] Ivanic, J. Direct Configuration Interaction and Multiconfigurational Self-Consistent-Field Method for Multiple Active Spaces with Variable Occupations. I. Method. *J. Chem. Phys.* **2003**, *119*, 9634-9376.

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[20] Roskop, L.; Gordon, M. S. Quasi-Degenerate Second-Order Perturbation Theory for Occupation Restricted Multiple Active Space Self-Consistent-Field Reference Functions. *J. Chem. Phys.* **2011**, *135*, 044101.

For systems **A-L**, ORMAS active spaces contained all valence π orbitals & electrons on the cyanine π backbone from one end nitrogen atom to the other, thus representing (14*e*, 13*o*) reference spaces. To illustrate, for the parent Cy9 species **A**, the $DET/$ORMAS GAMESS input specifications were:

```
$det   ncore=110 nels=14 nact=13 nstate=3 wstate(1)=1,1 $end
$ormas nspace=3 mstart(1)=111,117,119 mine(1)=10,0,0 maxe(1)=12,4,2 $end
```

For systems **M-O**, ORMAS active spaces were augmented by addition of the six valence π electrons & orbitals on the aromatic system directly attached to the central portion of the cyanine backbone, thus producing (20*e*, 19*o*) reference spaces. To illustrate, for the aryl-fused system **M** (**FNIR-1072**), the $DET/$ORMAS specifications were:

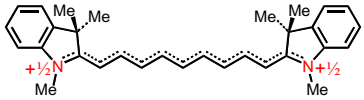
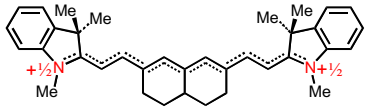
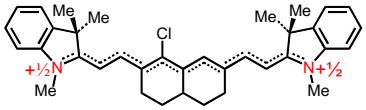
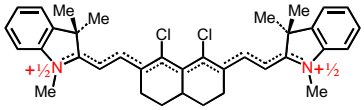
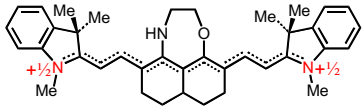
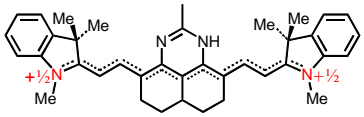
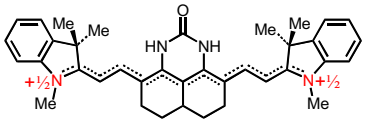
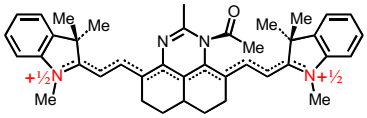
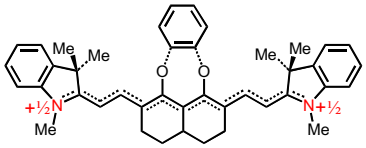
```
$det   ncore=144 nels=20 nact=19 nstate=3 wstate(1)=1,1 $end
$ormas nspace=3 mstart(1)=145,154,156 mine(1)=16,0,0 maxe(1)=18,4,2 $end
```

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 wave functions via perturbation theory (1s orbitals were kept core). All calculations were performed in solvent (water) phases via the polarized continuum model (PCM)[21,22,23] approach for

[21] Miertus, S.; Scrocco, E.; Tomasi, J. Electrostatic Interaction of a Solute with a Continuum. A direct utilization of Ab Initio Molecular Potentials for the Prevision of Solvent Effects. *J. Chem. Phys.* **1981**, *55*, 117-129.
[22] Li, H.; Jensen, J. H. Improving the Efficiency and Convergence of Geometry Optimization with the Polarizable Continuum Model: New Energy Gradients and Molecular Surface Tessellation. *J. Comput. Chem.*, **2004**, *25*, 1449-1462.
[23] Tomasi, J.; Mennucci, B.; Cammi, R. Quantum Mechanical Continuum Solvation Models. *Chem. Rev.*, **2005**, *105*, 2999-3094.

the DFT,[24] TDDFT,[25] ORMAS,[22] and ORMAS-PT2 methods. In all cases a high density of tesserae was used (NTSALL = 960 in $TESCAV).

Table SN1.1. Computed absorbance/emission energies (nm) vs. experimental (if available) for non-aryl-fused Cy9 species. Water solvent effects included via Polarizable Continuum Model (PCM). Experimental values in MeOH unless otherwise noted.

System		TDDFT-B3LYP-PCM	ORMAS-PT2-PCM	Experimental
A		653/798	929/957	855/880[26] (EtOH)
B		669/815	923/946	?
C		688/843	949/976	?
D		717/895	982/1061	?
E		598/712	704/780	?
F		599/693	712/757	?
G		625/732	808/844	?
H		644/834	848/983	?
I		666/797	933/960	866/896 (MeOH)

[24] Li, H. Quantum Mechanical/Molecular Mechanical/Continuum Style Solvation Model: Linear Response Theory, Variational Treatment, and Nuclear Gradients. *J. Chem. Phys*., **2009**, *131*, 184103.

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[26] Mostovnikov, V. A.; Rubinov, A. N.; Al'perovich, M. A.; Avdeeva, V. I.; Levkoev, I. I.; Loiko, M. M., Dependence of the Luminescence And Generation Properties of Solutions of Polymethine Dyes on Their Structure. *J. Appl. Spectrosc.* **1974,** *20*, 31-35. (measured in EtOH)

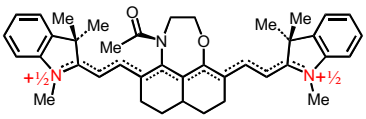
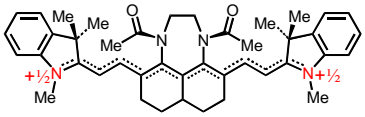
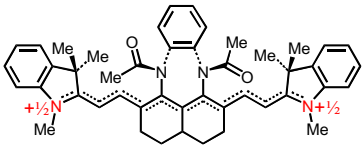
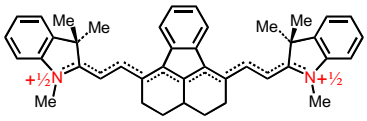
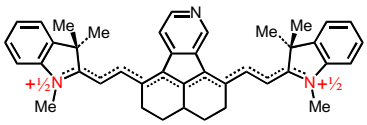
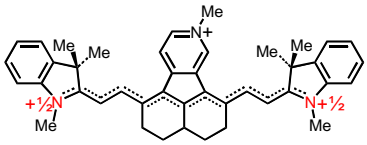
J		684/828	947/980	?
K		711/869	994/1027	?
L		722/888	1062/1091	?

Table SN1.2. Computed absorbance/emission energies (nm) vs. experimental (if available) for aryl-fused Cy9 species. Water solvent effects included via Polarizable Continuum Model (PCM).

System		TDDFT-B3LYP-PCM	ORMAS-PT2-PCM	Experimental
M		835/1072	1035/1074	1072/1103 (MeOH)
N		844/1090	1045/1072	?
O		973/1282	1108/1237	?

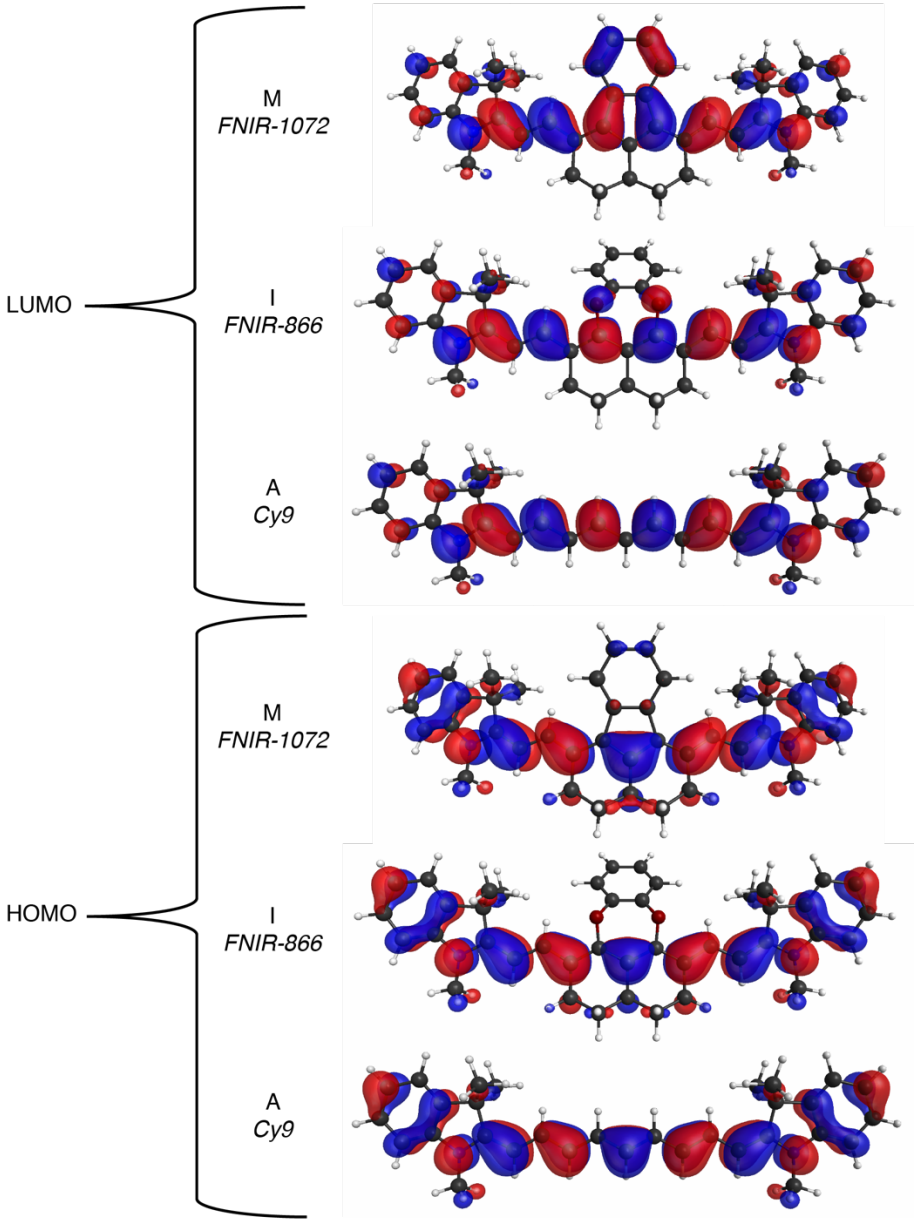
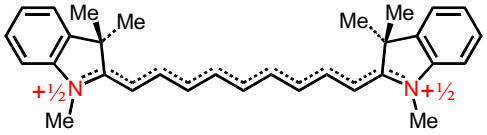


Figure SN1.1
Orbital diagrams

B3LYP-PCM HOMO and LUMO plots for **A** (**Cy9**), **I** (**FNIR-866**), and **M** (**FNIR-1072**; contour values = 0.02 (electron/bohr^3)$^{1/2}$.

Data at ground state optimized geometries: B3LYP-PCM & TDDFT-B3LYP-PCM energies (hartree) & wave function data, ORMAS-PT2-PCM energies (hartree), and B3LYP-PCM optimized geometries (Å)

A



E(B3LYP-PCM): S0 = –1310.842365
E(HOMO) = –0.1768; E(LUMO) = –0.1071

E(TDDFT-B3LYP-PCM): S1 = –1310.783573*
Oscillator strength S0 → S1 = 3.2745*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
117	118	0.997926	-0.094642
116	119	-0.096370	-0.028303
115	122	-0.033034	-0.013797

E(ORMAS-PT2-PCM): S0 = –1307.329274
E(ORMAS-PT2-PCM): S1 = –1307.280251*

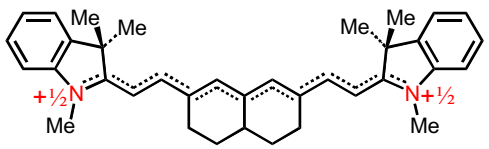
Optimized B3LYP-PCM geometry:

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1156665462	-0.0848476534	-0.5423064802
C	6.0	-1.1308850586	-0.0923743061	-1.1780492010
C	6.0	3.8140224174	-0.0603731874	-1.2050690556
C	6.0	-2.3407766887	-0.1020959269	-0.4880041731
C	6.0	5.0315969047	-0.0520274989	-0.5286454122
H	1.0	-2.2896094709	-0.1038081163	0.5977235209
H	1.0	4.9922439256	-0.0515406410	0.5576184368
C	6.0	-3.5932339870	-0.1094353960	-1.1212277836
C	6.0	6.2768874540	-0.0440662694	-1.1757659757
H	1.0	-3.5804878619	-0.1060072838	-2.2080357119
H	1.0	6.2524234880	-0.0458736574	-2.2623381565
C	6.0	-4.8396734378	-0.1210658871	-0.5024304541
C	6.0	7.5302465731	-0.0345811436	-0.5710112474
N	7.0	-5.9955061366	-0.1261635184	-1.2225264029
N	7.0	8.6779715904	-0.0233980445	-1.3039593357
C	6.0	-6.0541707831	-0.1185148112	-2.6801915162
C	6.0	8.7200322488	-0.0172096992	-2.7622562640
H	1.0	-7.0949233578	-0.1188278086	-2.9983308774
H	1.0	9.7560087029	0.0282542022	-3.0927258805

H	1.0	-5.5614507615	-1.0078826638	-3.0857949700
H	1.0	8.2610475108	-0.9275563454	-3.1611387855
H	1.0	-5.5655009818	0.7774935961	-3.0757895860
H	1.0	8.1890136474	0.8562996370	-3.1531301173
C	6.0	-7.1303571391	-0.1410110336	-0.3839732398
C	6.0	9.8222041696	-0.0218700467	-0.4781236079
C	6.0	-8.4791866245	-0.1510190465	-0.7344718263
C	6.0	11.1672200259	-0.0162259842	-0.8431191414
H	1.0	-8.8091416841	-0.1482504994	-1.7677729080
H	1.0	11.4858237875	-0.0138601179	-1.8799687447
C	6.0	-9.4143083029	-0.1654731172	0.3076995060
C	6.0	12.1136599531	-0.0148954364	0.1889732702
H	1.0	-10.4734002685	-0.1735660318	0.0654998148
H	1.0	13.1701292678	-0.0106372068	-0.0643812611
C	6.0	-9.0082135530	-0.1696913747	1.6460493019
C	6.0	11.7221411910	-0.0194406294	1.5317211756
H	1.0	-9.7528426682	-0.1810486241	2.4367363080
H	1.0	12.4753525178	-0.0183353372	2.3143262875
C	6.0	-7.6438842042	-0.1593465367	1.9743370588
C	6.0	10.3614937046	-0.0260800925	1.8746299854
H	1.0	-7.3324779172	-0.1626801369	3.0157537319
H	1.0	10.0611214594	-0.0302677866	2.9192586844
C	6.0	-6.7067602283	-0.1450011864	0.9495892138
C	6.0	9.4133780574	-0.0277035837	0.8600508475
C	6.0	-5.1866389169	-0.1315847745	0.9965057496
C	6.0	7.8938651713	-0.0357676735	0.9238447450
C	6.0	-4.6572922920	-1.4077163621	1.6962711229
C	6.0	7.3905521539	-1.3172977995	1.6328894373
C	6.0	-4.6801581269	1.1471182746	1.7085692014
C	6.0	7.3769167503	1.2377234360	1.6377524704
H	1.0	-5.0049050155	-2.3100694164	1.1830725521
H	1.0	7.7457356460	-2.2160628537	1.1185926832
H	1.0	-5.0441293344	2.0479542460	1.2041190789
H	1.0	7.7228338354	2.1421708150	1.1271069002
H	1.0	-5.0248921575	-1.4373917428	2.7276103340
H	1.0	7.7692432554	-1.3387714673	2.6603972946
H	1.0	-5.0479624952	1.1605012022	2.7401920826
H	1.0	7.7550283002	1.2590626034	2.6654799777
H	1.0	-3.5643243443	-1.4284515285	1.7258123048
H	1.0	6.2983709787	-1.3535669499	1.6739594851
H	1.0	-3.5877409798	1.1869067416	1.7381825427
H	1.0	6.2843719261	1.2625259292	1.6784639671
H	1.0	0.1296122434	-0.0859633325	0.5488330054
H	1.0	-1.1540475946	-0.0908536598	-2.2678390881
H	1.0	3.8253863459	-0.0604042195	-2.2950714498
C	6.0	1.3415051985	-0.0761450478	-1.2099806909
C	6.0	2.5745615358	-0.0684943949	-0.5556730551
H	1.0	2.5720322951	-0.0688281110	0.5355491851
H	1.0	1.3358204332	-0.0754423230	-2.3000758435

B



E(B3LYP-PCM): S0 = –1504.878260
E(HOMO) = –0.1715; E(LUMO) = –0.1037

E(TDDFT-B3LYP-PCM): S1 = –1504.810103*
Oscillator strength S0 → S1 = 2.8497*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
133	136	0.066541	0.027063
135	136	-1.007348	0.186583
134	137	0.106952	0.026197
133	140	0.036538	0.013039

E(ORMAS-PT2-PCM): S0 = –1500.849354
E(ORMAS-PT2-PCM): S1 = –1500.799995*

Optimized B3LYP-PCM geometry:

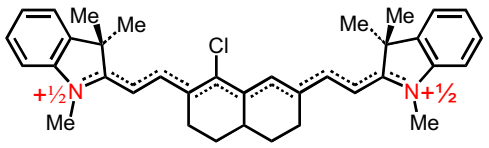
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1279994631	0.0505236628	-1.0929828254
C	6.0	-1.1394658772	0.0331491171	-1.7015278843
C	6.0	3.8173057955	0.0669055588	-1.7300586212
C	6.0	-2.2702198931	-0.0237339419	-0.8793730237
C	6.0	4.9578787739	0.0289862479	-0.9206102127
H	1.0	-2.0704071758	-0.0350402932	0.1884410867
H	1.0	4.7696492684	0.0195347088	0.1493131755
C	6.0	-3.6056477711	-0.0783874168	-1.3090770658
C	6.0	6.2891855673	-0.0090919306	-1.3646916094
H	1.0	-3.7844091681	-0.0821001389	-2.3793772025
H	1.0	6.4562913361	-0.0155986267	-2.4368403582
C	6.0	-4.7295689192	-0.1313994629	-0.4899058187
C	6.0	7.4225169289	-0.0431112342	-0.5576639863
N	7.0	-5.9908766464	-0.1800245731	-1.0054371070
N	7.0	8.6789803996	-0.0753452281	-1.0863658502
C	6.0	-6.2906306735	-0.1879084710	-2.4328463378
C	6.0	8.9627178792	-0.0803117252	-2.5170104487
H	1.0	-7.3683396712	-0.2399261504	-2.5768131945
H	1.0	10.0397503670	-0.1004416413	-2.6739825032
H	1.0	-5.8290690434	-1.0571732517	-2.9119493263
H	1.0	8.5211095149	-0.9643232625	-2.9880394039
H	1.0	-5.9149978195	0.7254590943	-2.9052004052

H	1.0	8.5546812155	0.8200105897	-2.9873260229
C	6.0	-6.9679309517	-0.2180909367	0.0112574012
C	6.0	9.6668688664	-0.1009723613	-0.0798300938
C	6.0	-8.3559880292	-0.2667905029	-0.1052708546
C	6.0	11.0541247735	-0.1350351303	-0.2102816673
H	1.0	-8.8560626065	-0.2801264030	-1.0678227109
H	1.0	11.5446484012	-0.1458691676	-1.1778014777
C	6.0	-9.1010655872	-0.2969737687	1.0803091924
C	6.0	11.8115002956	-0.1547938524	0.9677370766
H	1.0	-10.1852455492	-0.3347394617	1.0209117800
H	1.0	12.8953525622	-0.1813024655	0.8973998378
C	6.0	-8.4750825063	-0.2798148052	2.3310313145
C	6.0	11.1981747049	-0.1415305695	2.2248086997
H	1.0	-9.0750088039	-0.3046414808	3.2361999648
H	1.0	11.8074356632	-0.1577904894	3.1239173003
C	6.0	-7.0759325825	-0.2306386044	2.4232398915
C	6.0	9.7996311831	-0.1076572198	2.3311096224
H	1.0	-6.5924061770	-0.2174292624	3.3967620623
H	1.0	9.3255727187	-0.0977940681	3.3093221124
C	6.0	-6.3265988843	-0.1989539148	1.2548407253
C	6.0	9.0381757241	-0.0869516124	1.1703735675
C	6.0	-4.8209110085	-0.1440242419	1.0465760151
C	6.0	7.5297681151	-0.0503601248	0.9775964997
C	6.0	-4.1512626055	-1.4043639183	1.6492714551
C	6.0	6.8816419403	-1.3166685875	1.5910603412
C	6.0	-4.2395989496	1.1497511721	1.6688161958
C	6.0	6.9400937458	1.2387027132	1.6017893612
H	1.0	-4.5676728305	-2.3169526968	1.2107595457
H	1.0	7.3041798959	-2.2254410364	1.1504326547
H	1.0	-4.7053228237	2.0390210971	1.2319612031
H	1.0	7.3951840177	2.1315300167	1.1609943943
H	1.0	-4.3303052874	-1.4314373453	2.7295515906
H	1.0	7.0726652628	-1.3386192331	2.6693911460
H	1.0	-4.4346277518	1.1560068994	2.7465897382
H	1.0	7.1414400220	1.2481338864	2.6783763615
H	1.0	-3.0699762728	-1.4070072697	1.4858523584
H	1.0	5.7987023378	-1.3329010363	1.4396077182
H	1.0	-3.1583947757	1.2202607457	1.5215262340
H	1.0	5.8574384929	1.2993382929	1.4606836102
H	1.0	0.1700061050	0.0515085734	-0.0036222497
C	6.0	1.3383908857	0.0517490127	-1.7947667616
C	6.0	2.5566464450	0.0681153436	-1.1072206192
H	1.0	2.5268573181	0.0700332683	-0.0174498085
C	6.0	1.3294988898	0.0313277688	-3.3155609014
C	6.0	-1.2161278799	0.0564067951	-3.2174392310
C	6.0	3.8757886653	0.0863751951	-3.2469172861
C	6.0	2.6038397933	0.6946407212	-3.8615450768
C	6.0	0.0413409707	0.6806274202	-3.8456711608
H	1.0	4.0094152624	-0.9396267875	-3.6223965116
H	1.0	4.7507363218	0.6519672982	-3.5879766352
H	1.0	-1.3428778640	-0.9698959486	-3.5944589837
H	1.0	-2.1014429966	0.6131790782	-3.5460868636

H	1.0	1.3331774068	-1.0230429497	-3.6409196374
H	1.0	2.6369685248	0.5966685110	-4.9533760029
H	1.0	2.5713177923	1.7698519471	-3.6361328250
H	1.0	-0.0033065026	0.5840878447	-4.9371910344
H	1.0	0.0640608809	1.7557767313	-3.6186933026

C



E(B3LYP-PCM): S0 = –1964.402271
E(HOMO) = –0.1752; E(LUMO) = –0.1097

E(TDDFT-B3LYP-PCM): S1 = –1964.336012*
Oscillator strength S0 → S1 = 2.8005*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
141	144	0.061583	0.026028
143	144	1.009109	-0.193499
142	145	-0.105487	-0.027132
141	148	0.035539	0.013263

E(ORMAS-PT2-PCM): S0 = –1959.878798
E(ORMAS-PT2-PCM): S1 = –1959.830794*

Optimized B3LYP-PCM geometry:

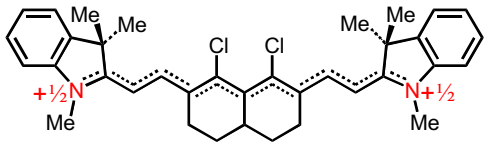
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1431286863	0.2820489287	-0.9134880701
C	6.0	-1.1395537006	0.2003279287	-1.5066551529
C	6.0	3.8446786104	0.2006042806	-1.6501928128
C	6.0	-2.3103795080	0.1213196644	-0.7458353149
C	6.0	5.0114013387	0.1418018423	-0.8714415787
H	1.0	-2.1934358142	0.1654670072	0.3285015162
H	1.0	4.8576274403	0.1820581546	0.2028514544
C	6.0	-3.6095125181	-0.0339497262	-1.2545902021
C	6.0	6.3180523874	0.0196641897	-1.3577432907
H	1.0	-3.7303088996	-0.1006633229	-2.3298721580
H	1.0	6.4471318956	-0.0329227371	-2.4335936422
C	6.0	-4.7706909715	-0.1272088361	-0.4896517028
C	6.0	7.4775459814	-0.0516481998	-0.5838745694
N	7.0	-5.9965600518	-0.2770288571	-1.0637249653
N	7.0	8.7082616421	-0.1655436546	-1.1495786418
C	6.0	-6.2239320801	-0.3432503885	-2.5029115513
C	6.0	8.9476992838	-0.2150622641	-2.5883995989
H	1.0	-7.2937961799	-0.3878619210	-2.6990714822
H	1.0	10.0193379959	-0.2466464113	-2.7766277498
H	1.0	-5.7487605597	-1.2347155210	-2.9253828627
H	1.0	8.4855911806	-1.1081691417	-3.0209609012
H	1.0	-5.8161013101	0.5479641998	-2.9894126155

H	1.0	8.5332146920	0.6760397080	-3.0690982522
C	6.0	-7.0186422995	-0.3612953596	-0.0945021673
C	6.0	9.7264738356	-0.2301850673	-0.1731482563
C	6.0	-8.3903223360	-0.5282515228	-0.2767257434
C	6.0	11.1031660103	-0.3572934113	-0.3474180117
H	1.0	-8.8375539188	-0.6171724353	-1.2610354949
H	1.0	11.5599379522	-0.4237375633	-1.3290756235
C	6.0	-9.1899769744	-0.5812839425	0.8716759449
C	6.0	11.8955037364	-0.3987001897	0.8064338347
H	1.0	-10.2628263766	-0.7118385977	0.7613437543
H	1.0	12.9723216449	-0.4982135047	0.7031769161
C	6.0	-8.6320158815	-0.4710953360	2.1496950190
C	6.0	11.3250084956	-0.3163315091	2.0811484875
H	1.0	-9.2731761756	-0.5155666569	3.0253167102
H	1.0	11.9609012469	-0.3514851487	2.9610043222
C	6.0	-7.2480552211	-0.3052910087	2.3081410221
C	6.0	9.9361239335	-0.1898690122	2.2312340403
H	1.0	-6.8177467003	-0.2222448229	3.3029488040
H	1.0	9.4962982294	-0.1278250078	3.2233411067
C	6.0	-6.4445591798	-0.2520196646	1.1769380850
C	6.0	9.1399116626	-0.1479939213	1.0943952778
C	6.0	-4.9383568410	-0.0913820976	1.0395489870
C	6.0	7.6315212775	-0.0255231161	0.9460619745
C	6.0	-4.2125426837	-1.2750077892	1.7273187976
C	6.0	6.9290578328	-1.2342308070	1.6142053092
C	6.0	-4.4862867035	1.2653054171	1.6352576161
C	6.0	7.1374837882	1.3130130061	1.5496950271
H	1.0	-4.5310078864	-2.2318518782	1.3011859095
H	1.0	7.2832613543	-2.1787575073	1.1889066116
H	1.0	-5.0017503897	2.0994281124	1.1483647979
H	1.0	7.6318357496	2.1656654286	1.0732176611
H	1.0	-4.4547364711	-1.2794001852	2.7954255178
H	1.0	7.1518790851	-1.2373267236	2.6864865842
H	1.0	-4.7259818769	1.2914906972	2.7035546204
H	1.0	7.3696271804	1.3367124781	2.6196658857
H	1.0	-3.1261943503	-1.1996335014	1.6281864626
H	1.0	5.8430713254	-1.1893850611	1.4949754726
H	1.0	-3.4088345652	1.4171907845	1.5263794835
H	1.0	6.0568496054	1.4338248340	1.4353386693
C	6.0	1.3612827008	0.2502756648	-1.6129087855
C	6.0	2.6141616430	0.2718768256	-0.9814760877
H	1.0	2.6438981311	0.3198824200	0.1028285168
C	6.0	1.3193467836	0.1412854413	-3.1368921601
C	6.0	-1.2006823087	0.1556418478	-3.0271910083
C	6.0	3.8654806128	0.1641513351	-3.1645300869
C	6.0	2.5815695465	0.7635312771	-3.7528591290
C	6.0	0.0361663316	0.7673030266	-3.6876031236
H	1.0	3.9799978513	-0.8752866340	-3.5077828477
H	1.0	4.7349845321	0.7103050146	-3.5487363819
H	1.0	-1.3174196142	-0.8874022838	-3.3575069530
H	1.0	-2.0941462570	0.6889422752	-3.3697203987
H	1.0	1.3108433292	-0.9310272030	-3.3942381000

H	1.0	2.5658981378	0.6177905157	-4.8395264168
H	1.0	2.5696849641	1.8475486785	-3.5731546383
H	1.0	-0.0133407038	0.6236563562	-4.7733791254
H	1.0	0.0543558209	1.8507475805	-3.5052020658
CL	17.0	0.2258569229	0.4038117301	0.8634503013

D



E(B3LYP-PCM): S0 = –2423.910084
E(HOMO) = –0.1783; E(LUMO) = –0.1150

E(TDDFT-B3LYP-PCM): S1 = –2423.846510*
Oscillator strength S0 → S1 = 2.6729*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
149	152	0.048867	0.024504
151	152	1.010909	-0.197141
150	153	0.099593	0.025823
149	156	-0.030816	-0.012103

E(ORMAS-PT2-PCM): S0 = –2418.893709
E(ORMAS-PT2-PCM): S1 = –2418.847323*

Optimized B3LYP-PCM geometry:

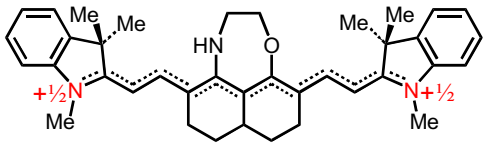
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0834142358	0.1633720716	-0.5302046816
C	6.0	-1.1543921093	0.3222904913	-1.1893375700
C	6.0	3.8318226024	0.0376416923	-1.2687159917
C	6.0	-2.3816191024	0.0561810922	-0.5540396309
C	6.0	5.0844430742	0.1444909743	-0.6534967674
H	1.0	-2.3379437799	-0.2881871217	0.4694675764
H	1.0	5.1004331546	0.5616016784	0.3441467186
C	6.0	-3.6381798218	0.1977280371	-1.1459869064
C	6.0	6.3075868123	-0.2711188881	-1.1997204735
H	1.0	-3.6853800149	0.5287892954	-2.1770308807
H	1.0	6.3006674410	-0.7229214486	-2.1848414226
C	6.0	-4.8631635525	-0.0550676683	-0.5174948133
C	6.0	7.5487928596	-0.1711312884	-0.5716226311
N	7.0	-6.0396659075	0.0910364769	-1.1750490521
N	7.0	8.6885482726	-0.6086109090	-1.1725792890
C	6.0	-6.1571712422	0.4997069590	-2.5726985456
C	6.0	8.7347152857	-1.2171520609	-2.4983097055
H	1.0	-7.2065062025	0.5018552174	-2.8605917877
H	1.0	9.7664529385	-1.4533197256	-2.7516840623
H	1.0	-5.6163941330	-0.2005820980	-3.2157886232
H	1.0	8.1466137076	-2.1400679026	-2.5117874259
H	1.0	-5.7508064184	1.5067245433	-2.7079944237

H	1.0	8.3386944166	-0.5237717712	-3.2464763413
C	6.0	-7.1437615888	-0.1925065176	-0.3395462350
C	6.0	9.8199868177	-0.4094505286	-0.3527239447
C	6.0	-8.5038702191	-0.1518157781	-0.6393724949
C	6.0	11.1539902190	-0.7231928875	-0.6065179690
H	1.0	-8.8745315882	0.1237988762	-1.6207906280
H	1.0	11.4742120859	-1.1892634251	-1.5322292702
C	6.0	-9.3961434486	-0.4834244168	0.3870854802
C	6.0	12.0874851112	-0.4130772001	0.3898037820
H	1.0	-10.4634385026	-0.4610556274	0.1860730730
H	1.0	13.1352805666	-0.6454619879	0.2213088653
C	6.0	-8.9367438358	-0.8401936387	1.6597866173
C	6.0	11.6938316646	0.1870740082	1.5907079679
H	1.0	-9.6495857038	-1.0927913952	2.4393458439
H	1.0	12.4373636979	0.4174044853	2.3481846059
C	6.0	-7.5624279940	-0.8737606498	1.9370137710
C	6.0	10.3446270793	0.4927232066	1.8235719309
H	1.0	-7.2108440922	-1.1513180937	2.9273469133
H	1.0	10.0427798734	0.9587013926	2.7581144779
C	6.0	-6.6675178100	-0.5461081522	0.9269424498
C	6.0	9.4094360077	0.1900859740	0.8428490825
C	6.0	-5.1481546010	-0.4957024094	0.9274645969
C	6.0	7.9035390490	0.4002777035	0.8122144192
C	6.0	-4.5686367724	-1.9016428023	1.2288885539
C	6.0	7.2305841340	-0.3986795861	1.9566534120
C	6.0	-4.6450522931	0.5502142447	1.9543969109
C	6.0	7.5715872626	1.9104156369	0.9116246688
H	1.0	-4.9222116533	-2.6371586174	0.4994075176
H	1.0	7.4510661557	-1.4675314741	1.8719029935
H	1.0	-5.0343510024	1.5467742850	1.7228333739
H	1.0	8.0481117464	2.4707938020	0.1008908844
H	1.0	-4.8974291986	-2.2196472039	2.2235838667
H	1.0	7.6134063189	-0.0455072968	2.9200272801
H	1.0	-4.9905524075	0.2715054604	2.9552431853
H	1.0	7.9451215353	2.3024563056	1.8634637096
H	1.0	-3.4752073740	-1.9030168518	1.2175650716
H	1.0	6.1445113867	-0.2708494359	1.9593925271
H	1.0	-3.5530566076	0.6043484808	1.9770465013
H	1.0	6.4941527541	2.0938752940	0.8693478109
C	6.0	1.3441619436	0.2345549381	-1.1751469431
C	6.0	2.6240670067	0.3652776036	-0.6006553449
C	6.0	1.2533158602	0.1424891521	-2.7105670237
C	6.0	-1.1746941738	0.7910489966	-2.6377450807
C	6.0	3.6912823712	-0.4555819944	-2.6960606436
C	6.0	2.5978481271	0.3436542815	-3.4040311688
C	6.0	0.2026478846	1.1540436549	-3.1869349281
H	1.0	3.4421992893	-1.5269227483	-2.7146372118
H	1.0	4.6374461094	-0.3418841743	-3.2309378902
H	1.0	-1.6113531256	-0.0098536045	-3.2517138460
H	1.0	-1.8524705011	1.6490988333	-2.7300882774
H	1.0	0.8920720304	-0.8676857858	-2.9598467986
H	1.0	2.5090657665	0.0357354214	-4.4521033770

H	1.0	2.8682726504	1.4083360330	-3.3997274067
H	1.0	0.1705018389	1.1716150000	-4.2829353542
H	1.0	0.4992447162	2.1574535441	-2.8556008778
CL	17.0	0.0165565580	-0.3339803990	1.1761892788
CL	17.0	2.7789714780	1.0613172014	1.0279378215

E



E(B3LYP-PCM): S0 = –1712.744782
E(HOMO) = –0.1739; E(LUMO) = –0.0880

E(TDDFT-B3LYP-PCM): S1 = –1712.668530*
Oscillator strength S0 → S1 = 2.1730*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
149	151	-0.072744	-0.004806
150	151	-0.996141	0.096498
148	152	-0.030446	-0.010221
149	152	-0.070960	0.006072
148	155	0.033262	0.009637

E(ORMAS-PT2-PCM): S0 = –1708.234260
E(ORMAS-PT2-PCM): S1 = –1708.169533*

Optimized B3LYP-PCM geometry:

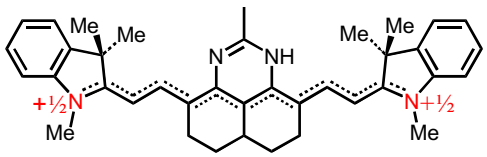
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1230954338	-0.9052595740	-0.6764427277
C	6.0	-1.0013565633	-0.2348360214	-1.2894422693
C	6.0	3.9049058397	-1.0942214705	-1.3700263297
C	6.0	-2.2433629829	-0.2863445533	-0.6807378800
C	6.0	5.0538261335	-0.7107188817	-0.7080261063
H	1.0	-2.3139300347	-0.8990017971	0.2083698422
H	1.0	4.9670473054	-0.4489220616	0.3419626653
C	6.0	-3.4118965901	0.3948363296	-1.1066051729
C	6.0	6.3340748100	-0.5751816883	-1.3169942056
H	1.0	-3.3248592065	1.0539438799	-1.9635660571
H	1.0	6.4247213624	-0.9188964117	-2.3416146642
C	6.0	-4.6595418983	0.3080928600	-0.5175825425
C	6.0	7.4711731110	-0.0554576895	-0.7337903534
N	7.0	-5.7375921520	1.0101372372	-0.9970833474
N	7.0	8.6672239089	0.0104292289	-1.4082917784
C	6.0	-5.6772274978	1.9032646487	-2.1444522647
C	6.0	8.8539299803	-0.4606922256	-2.7717423367
H	1.0	-6.6695034929	2.3036734630	-2.3466351130
H	1.0	9.8940761588	-0.3238764739	-3.0635751864
H	1.0	-5.3312765349	1.3624038650	-3.0318292843
H	1.0	8.6059620453	-1.5251567220	-2.8454819282

H	1.0	-4.9943094429	2.7371148063	-1.9471722240
H	1.0	8.2170632307	0.1011054066	-3.4646753768
C	6.0	-6.8967192111	0.7633897772	-0.2391926509
C	6.0	9.6728554980	0.6048934412	-0.6247209960
C	6.0	-8.1808797490	1.2815667057	-0.4026440383
C	6.0	11.0063387061	0.8560132186	-0.9463956257
H	1.0	-8.4243339010	1.9824316481	-1.1944295741
H	1.0	11.4272015707	0.5943788355	-1.9116871870
C	6.0	-9.1671204367	0.8653031946	0.5009808564
C	6.0	11.8045439901	1.4674813846	0.0296721414
H	1.0	-10.1762112677	1.2546387190	0.3954310403
H	1.0	12.8469294249	1.6744394618	-0.1977017446
C	6.0	-8.8751220718	-0.0357734301	1.5294875120
C	6.0	11.2841490618	1.8142124955	1.2797680732
H	1.0	-9.6565092665	-0.3441717625	2.2181658877
H	1.0	11.9217112498	2.2881514940	2.0206635738
C	6.0	-7.5746579255	-0.5440502472	1.6755760267
C	6.0	9.9385916307	1.5509982438	1.5824565895
H	1.0	-7.3494897132	-1.2441185978	2.4765271370
H	1.0	9.5354315590	1.8211132469	2.5555095261
C	6.0	-6.5884820260	-0.1396657406	0.7862811551
C	6.0	9.1376496108	0.9457043187	0.6237879976
C	6.0	-5.1159003575	-0.5178988298	0.7014384525
C	6.0	7.6702834636	0.5426651305	0.6731051259
C	6.0	-4.9658517767	-2.0385371990	0.4504104692
C	6.0	7.4468802135	-0.5087618933	1.7871306815
C	6.0	-4.3815714941	-0.0927976568	1.9966609542
C	6.0	6.7764355853	1.7865988275	0.8957191551
H	1.0	-5.4975848728	-2.3396098122	-0.4582617763
H	1.0	8.0685689972	-1.3947824511	1.6225073278
H	1.0	-4.4762045777	0.9849671708	2.1652880350
H	1.0	6.9358685200	2.5288630440	0.1068053802
H	1.0	-5.3892323023	-2.5949053332	1.2940122948
H	1.0	7.7155353034	-0.0777442820	2.7578544450
H	1.0	-4.8226551079	-0.6120537518	2.8546021062
H	1.0	7.0230173359	2.2511653797	1.8568515647
H	1.0	-3.9164415293	-2.3277861419	0.3448229501
H	1.0	6.4025143195	-0.8283676841	1.8415707055
H	1.0	-3.3175404419	-0.3428611787	1.9620944505
H	1.0	5.7148419561	1.5228997238	0.9089863785
C	6.0	1.4123316040	-0.9277466004	-1.2491450790
C	6.0	2.6588063352	-1.2663687858	-0.6227541380
C	6.0	1.5618211998	-0.4470597715	-2.7043635216
C	6.0	-0.7653030307	0.4887846780	-2.5941618124
C	6.0	3.9142687361	-1.2908657216	-2.8747710592
O	8.0	-0.2079288738	-1.4405024308	0.5234788536
N	7.0	2.8373677474	-1.7055742618	0.6469323623
C	6.0	0.2284171547	-0.3071290671	-3.4358275904
C	6.0	2.5026400077	-1.4070889555	-3.4474234501
H	1.0	-0.3732401733	1.5029053631	-2.4202629824
H	1.0	-1.7071130050	0.6065742424	-3.1378684530
H	1.0	0.4003241765	0.1805113549	-4.4028825299

H	1.0	-0.1885330383	-1.3025727751	-3.6444894926
H	1.0	2.0381069019	0.5473801255	-2.6956143152
H	1.0	2.5146344928	-1.1712853633	-4.5184322197
H	1.0	2.1171111596	-2.4302168183	-3.3454007137
H	1.0	4.4215745731	-0.4350043159	-3.3406985332
H	1.0	4.5119200511	-2.1763826632	-3.1353430578
C	6.0	0.5621318152	-2.4766006258	1.1241511370
C	6.0	1.8540736197	-1.9165336288	1.6915739982
H	1.0	3.7580580829	-2.0733517689	0.8400271566
H	1.0	2.2865733401	-2.6232666672	2.4045850548
H	1.0	1.6327265358	-0.9865343310	2.2305679051
H	1.0	-0.0683315948	-2.8621189984	1.9277417346
H	1.0	0.7586734612	-3.2756084479	0.4002867963

F



E(B3LYP-PCM): S0 = –1691.723972
E(HOMO) = –0.1747; E(LUMO) = –0.0898

E(TDDFT-B3LYP-PCM): S1 = –1691.647907*
Oscillator strength S0 → S1 = 2.2690*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
148	150	-0.041960	-0.000358
149	150	0.998639	-0.101877
146	151	0.041670	0.018554
148	151	0.042922	-0.010459
148	152	-0.053400	-0.006235
147	155	0.034646	0.010747

E(ORMAS-PT2-PCM): S0 = –1687.262605
E(ORMAS-PT2-PCM): S1 = –1687.198567*

Optimized B3LYP-PCM geometry:

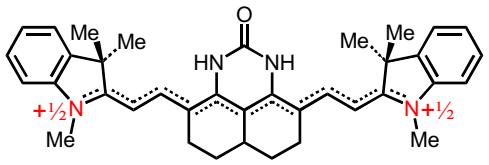
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1528705049	0.5764952637	-0.8849532929
C	6.0	-1.1544467023	0.4691464191	-1.4800962736
C	6.0	3.8325145684	0.2151169836	-1.5900442112
C	6.0	-2.2904573676	0.2960994492	-0.7104195046
C	6.0	5.0010496722	0.1573154346	-0.8506013864
H	1.0	-2.1771547941	0.2236005919	0.3671552370
H	1.0	4.8820184539	0.3136926516	0.2144007015
C	6.0	-3.6052411624	0.1390900382	-1.2210473593
C	6.0	6.2996509599	-0.0929294917	-1.3562472003
H	1.0	-3.7234558831	0.2072643666	-2.2965878364
H	1.0	6.3999265228	-0.2516405436	-2.4248871569
C	6.0	-4.7519471956	-0.1075359710	-0.4884081337
C	6.0	7.4586511307	-0.1643929193	-0.6036980161
N	7.0	-5.9779960181	-0.2434407114	-1.0895243246
N	7.0	8.6857661665	-0.3853129115	-1.1747467941
C	6.0	-6.1926134034	-0.1344289750	-2.5248044345
C	6.0	8.9011570166	-0.5373607208	-2.6059910319
H	1.0	-7.2547795780	-0.2363852550	-2.7428620339
H	1.0	9.9705311374	-0.5543566647	-2.8126823954
H	1.0	-5.6468240713	-0.9216477887	-3.0568163830

H	1.0	8.4546551508	-1.4688411306	-2.9726491225
H	1.0	-5.8534848372	0.8418788322	-2.8872415797
H	1.0	8.4578132856	0.3062674368	-3.1444367678
C	6.0	-6.9917677326	-0.5058520331	-0.1482509671
C	6.0	9.7045237300	-0.4535769984	-0.2058589807
C	6.0	-8.3555326426	-0.7116890613	-0.3538866011
C	6.0	11.0691381237	-0.6810187302	-0.3796594420
H	1.0	-8.8016580131	-0.6888306817	-1.3427604774
H	1.0	11.5069573841	-0.8466811843	-1.3585119329
C	6.0	-9.1509456448	-0.9540674928	0.7740993289
C	6.0	11.8740028427	-0.6953598390	0.7671698756
H	1.0	-10.2168682762	-1.1178927684	0.6408765955
H	1.0	12.9409235605	-0.8711374244	0.6594468473
C	6.0	-8.5991406604	-0.9886778392	2.0584368777
C	6.0	11.3289902954	-0.4916479852	2.0384211937
H	1.0	-9.2361279112	-1.1777158354	2.9177297770
H	1.0	11.9725468735	-0.5086709357	2.9133793193
C	6.0	-7.2235541440	-0.7803153743	2.2415757810
C	6.0	9.9515114006	-0.2674382742	2.1897382487
H	1.0	-6.7937219916	-0.8085351483	3.2399405933
H	1.0	9.5297761290	-0.1109875612	3.1796528978
C	6.0	-6.4255694279	-0.5406620123	1.1317338452
C	6.0	9.1434030774	-0.2502500033	1.0610303109
C	6.0	-4.9291867083	-0.2844841223	1.0313918242
C	6.0	7.6422478326	-0.0385337463	0.9211525228
C	6.0	-4.1419996206	-1.5071244534	1.5626807820
C	6.0	6.8738443416	-1.1442276872	1.6856797308
C	6.0	-4.5590886614	1.0034226150	1.8067117530
C	6.0	7.2516137353	1.3693971638	1.4345988998
H	1.0	-4.4052340055	-2.4128253277	1.0066714824
H	1.0	7.1627694690	-2.1385643559	1.3296375017
H	1.0	-5.1225530135	1.8629875532	1.4296769182
H	1.0	7.8032706080	2.1488723572	0.8987708283
H	1.0	-4.3855699085	-1.6709738744	2.6180158424
H	1.0	7.1078757272	-1.0827560987	2.7541356738
H	1.0	-4.7985348248	0.8754437581	2.8679412602
H	1.0	7.4937674145	1.4500456687	2.4999492313
H	1.0	-3.0610495734	-1.3610943893	1.4846475094
H	1.0	5.7916537819	-1.0391989089	1.5695724439
H	1.0	-3.4932347913	1.2347871625	1.7278557105
H	1.0	6.1819923360	1.5623777757	1.3147366245
C	6.0	1.3458922761	0.4146278525	-1.6058927501
C	6.0	2.5814583983	0.4426078535	-0.9125526710
C	6.0	1.2882036736	0.2067613926	-3.1057062684
C	6.0	-1.2305079070	0.4544320625	-2.9993248853
C	6.0	3.8116509409	0.0111555878	-3.0937131217
C	6.0	2.5975140142	0.6738674467	-3.7526942867
C	6.0	0.0592739731	0.9276254011	-3.6751528242
H	1.0	3.8092128099	-1.0652696373	-3.3262797351
H	1.0	4.7282549207	0.4145428984	-3.5388012331
H	1.0	-1.4723663784	-0.5630312046	-3.3420705335
H	1.0	-2.0620574408	1.0893134732	-3.3292084183

H	1.0	1.1748976474	-0.8720106128	-3.3050898184
H	1.0	2.5797539969	0.4476659437	-4.8252440936
H	1.0	2.6761560051	1.7656243782	-3.6538556423
H	1.0	-0.0051136164	0.7567982413	-4.7559728878
H	1.0	0.1822551998	2.0092907423	-3.5259016713
N	7.0	0.2915908758	0.8212930794	0.4696983698
N	7.0	2.6211385166	0.6691026901	0.4516473741
C	6.0	1.5054502761	0.8610371732	1.0931295030
C	6.0	1.4995723948	1.1432214775	2.5680799959
H	1.0	0.9290732773	0.3795164613	3.1093791613
H	1.0	1.0387517914	2.1162313485	2.7751590638
H	1.0	2.5257640538	1.1497603718	2.9370039969
H	1.0	-0.5306812471	1.0382026576	1.0179033762

G



E(B3LYP-PCM): S0 = –1727.650518
E(HOMO) = –0.1780; E(LUMO) = –0.0983

E(TDDFT-B3LYP-PCM): S1 = –1727.577621*
Oscillator strength S0 → S1 = 2.4186*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
149	150	-1.000868	0.120830
146	151	0.031005	0.016775
148	151	0.076231	-0.000195
147	154	0.036110	0.011589
148	155	-0.031601	-0.011166

E(ORMAS-PT2-PCM): S0 = –1723.147285
E(ORMAS-PT2-PCM): S1 = –1723.090926*

Optimized B3LYP-PCM geometry:

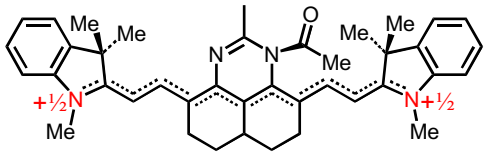
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1106817300	0.8824200878	-0.9359616949
C	6.0	-1.1611134115	0.5868654285	-1.5265975950
C	6.0	3.8164297074	0.6210097215	-1.5566745383
C	6.0	-2.3000854284	0.4144679655	-0.7508437683
C	6.0	4.9664513570	0.4638131682	-0.7942894696
H	1.0	-2.2045670413	0.4883204914	0.3277268563
H	1.0	4.8824739807	0.5365791989	0.2853563444
C	6.0	-3.5788712691	0.0833356349	-1.2534734379
C	6.0	6.2435206723	0.1486539310	-1.3113601160
H	1.0	-3.6799843034	0.0098958381	-2.3300770006
H	1.0	6.3328600042	0.0746047567	-2.3889886759
C	6.0	-4.7195404127	-0.1728112958	-0.5070096769
C	6.0	7.3957253532	-0.0917197802	-0.5775506079
N	7.0	-5.9079230241	-0.4945189866	-1.1021168224
N	7.0	8.5815755487	-0.3986042147	-1.1853817703
C	6.0	-6.0951517632	-0.6068862844	-2.5426289357
C	6.0	8.7543606306	-0.5072452358	-2.6279262519
H	1.0	-7.1128949743	-0.9333079722	-2.7500276688
H	1.0	9.7788713658	-0.8022957237	-2.8482651586
H	1.0	-5.4004622244	-1.3437284305	-2.9586256758

H	1.0	8.0765272778	-1.2643830345	-3.0354628757
H	1.0	-5.9274508768	0.3600051503	-3.0291325287
H	1.0	8.5517028366	0.4539061069	-3.1124705872
C	6.0	-6.9250709016	-0.7094642650	-0.1503482486
C	6.0	9.6108887475	-0.6035644930	-0.2445342456
C	6.0	-8.2636674543	-1.0420756292	-0.3531000870
C	6.0	10.9501721890	-0.9245030803	-0.4611769259
H	1.0	-8.6831397055	-1.1747871121	-1.3447827338
H	1.0	11.3599822912	-1.0555603282	-1.4571032304
C	6.0	-9.0684926495	-1.2003589306	0.7824525935
C	6.0	11.7686168783	-1.0737250750	0.6658406520
H	1.0	-10.1156443636	-1.4600884092	0.6537323399
H	1.0	12.8166036234	-1.3243760814	0.5262967440
C	6.0	-8.5488393661	-1.0305978417	2.0695197344
C	6.0	11.2614912091	-0.9062628166	1.9582311784
H	1.0	-9.1923913980	-1.1584002948	2.9351401418
H	1.0	11.9156314939	-1.0265823747	2.8169607160
C	6.0	-7.1986343930	-0.6928365725	2.2490699663
C	6.0	9.9100878803	-0.5815406694	2.1518350906
H	1.0	-6.7976081037	-0.5594139528	3.2507272030
H	1.0	9.5186239607	-0.4506931703	3.1576086258
C	6.0	-6.3912488293	-0.5328615583	1.1311295482
C	6.0	9.0891557246	-0.4313350991	1.0424914961
C	6.0	-4.9187328106	-0.1669837877	1.0198971842
C	6.0	7.6115945388	-0.0819782020	0.9470833388
C	6.0	-4.0452677266	-1.2385764412	1.7171710960
C	6.0	6.7585598388	-1.1626570983	1.6554643365
C	6.0	-4.6742929241	1.2369936315	1.6253063645
C	6.0	7.3579527474	1.3199947558	1.5533520555
H	1.0	-4.2078877498	-2.2265669284	1.2746398087
H	1.0	6.9283790715	-2.1493257499	1.2126852960
H	1.0	-5.2895881783	1.9925377876	1.1263804834
H	1.0	7.9602446558	2.0814253129	1.0475565987
H	1.0	-4.3095088502	-1.2915067811	2.7788913644
H	1.0	7.0350025186	-1.2106566567	2.7143039013
H	1.0	-4.9373335088	1.2289564430	2.6885738063
H	1.0	7.6314957356	1.3160093828	2.6139864993
H	1.0	-2.9796781214	-1.0031493608	1.6461198415
H	1.0	5.6894611880	-0.9404997944	1.5956088966
H	1.0	-3.6268219809	1.5392924468	1.5411137806
H	1.0	6.3065277484	1.6108850738	1.4790574570
C	6.0	1.3262953522	0.7295478829	-1.6293735876
C	6.0	2.5479565605	0.8996062153	-0.9509281243
C	6.0	1.3201893731	0.3450378725	-3.0951649734
C	6.0	-1.2103138488	0.3684305671	-3.0306295807
C	6.0	3.8508253318	0.4033589800	-3.0612817364
C	6.0	2.5846171698	0.8880134709	-3.7704230743
C	6.0	0.0404104127	0.8704579190	-3.7550391819
H	1.0	4.0039723409	-0.6657566899	-3.2726805010
H	1.0	4.7188626630	0.9230115665	-3.4848315045
H	1.0	-1.3509102891	-0.7028010634	-3.2399385399
H	1.0	-2.0904829514	0.8757023640	-3.4439466852

H	1.0	1.3271903413	-0.7543194252	-3.1816266119
H	1.0	2.6074442202	0.5768789911	-4.8213085674
H	1.0	2.5495716952	1.9861853166	-3.7583863175
H	1.0	0.0092466820	0.5588297065	-4.8055416122
H	1.0	0.0604652862	1.9690145219	-3.7434459496
N	7.0	2.4900033813	1.3110810005	0.3730239949
N	7.0	0.1792466090	1.2941345654	0.3874613133
C	6.0	1.3371290931	1.5660610858	1.0861045927
O	8.0	1.3411313951	1.9964424504	2.2330809202
H	1.0	3.3362092720	1.5771288661	0.8584813343
H	1.0	-0.6645196103	1.5461413553	0.8844310996

H



E(B3LYP-PCM): S0 = –1844.267126
E(HOMO) = –0.1753; E(LUMO) = –0.0986

E(TDDFT-B3LYP-PCM): S1 = –1844.196383*
Oscillator strength S0 → S1 = 2.2491*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
158	161	0.032630	0.024412
159	161	-0.043826	-0.001736
160	161	1.000607	-0.127547
157	162	0.033458	0.016876
159	162	0.051954	-0.001095
159	163	-0.041552	-0.003424
159	164	0.043737	0.009205
158	167	0.033842	0.011324

E(ORMAS-PT2-PCM): S0 = –1839.448813
E(ORMAS-PT2-PCM): S1 = –1839.395081*

Optimized B3LYP-PCM geometry:

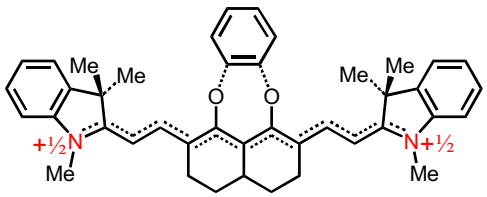
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1418289002	0.9522482344	-1.0255121700
C	6.0	-1.1600128768	0.7367198865	-1.5922024278
C	6.0	3.7634844250	0.2144144356	-1.6417187638
C	6.0	-2.2590306970	0.4622698488	-0.7895022858
C	6.0	4.9152518448	0.1044341664	-0.8738708102
H	1.0	-2.0925546463	0.3841452980	0.2792522629
H	1.0	4.7890984296	0.3233387175	0.1789484534
C	6.0	-3.5636930916	0.2038874018	-1.2688911875
C	6.0	6.1940581372	-0.2678445533	-1.3392604574
H	1.0	-3.7296726263	0.3223971260	-2.3341365388
H	1.0	6.2974433587	-0.5106875878	-2.3917285076
C	6.0	-4.6549656365	-0.1914604309	-0.5107004326
C	6.0	7.3403525014	-0.3547693863	-0.5623291551
N	7.0	-5.8835617575	-0.4020188581	-1.0743832344
N	7.0	8.5456818700	-0.7290902309	-1.0883218445
C	6.0	-6.1696120164	-0.2208775065	-2.4911366443
C	6.0	8.7497509583	-1.0729344700	-2.4892799864
H	1.0	-7.2257862262	-0.4097112717	-2.6768387994

H	1.0	9.7974582485	-1.3193946616	-2.6534075136
H	1.0	-5.5759221216	-0.9161872994	-3.0944953657
H	1.0	8.1371022782	-1.9384007353	-2.7629210993
H	1.0	-5.9387042513	0.8050823231	-2.7960038929
H	1.0	8.4825569256	-0.2271775801	-3.1314622193
C	6.0	-6.8298901341	-0.8199651311	-0.1175658881
C	6.0	9.5608790710	-0.7339760490	-0.1107634832
C	6.0	-8.1765258512	-1.1366712511	-0.2909397787
C	6.0	10.9106748243	-1.0543502311	-0.2465619929
H	1.0	-8.6616541573	-1.0877403653	-1.2601171173
H	1.0	11.3417450597	-1.3561568927	-1.1953876500
C	6.0	-8.8995659494	-1.5267220659	0.8437219691
C	6.0	11.7115944805	-0.9747331319	0.9001262652
H	1.0	-9.9509426628	-1.7795749563	0.7375512660
H	1.0	12.7676878851	-1.2182494534	0.8223371006
C	6.0	-8.2934091382	-1.5961287620	2.1021402259
C	6.0	11.1767657342	-0.5888063952	2.1331992926
H	1.0	-8.8746440815	-1.9016564898	2.9673967777
H	1.0	11.8180128762	-0.5345299458	3.0083384956
C	6.0	-6.9362067912	-1.2730400124	2.2523540238
C	6.0	9.8142645771	-0.2722480746	2.2463705178
H	1.0	-6.4669009330	-1.3278551283	3.2315242130
H	1.0	9.3998634656	0.0269171815	3.2060110224
C	6.0	-6.2090720213	-0.8857802115	1.1350965175
C	6.0	9.0103896475	-0.3468377185	1.1169175960
C	6.0	-4.7491765016	-0.4794097001	0.9996343693
C	6.0	7.5251910578	-0.0676157776	0.9395551293
C	6.0	-3.8239035294	-1.6475031169	1.4197198496
C	6.0	6.6923062790	-1.0322645815	1.8195788556
C	6.0	-4.4717963475	0.7852702229	1.8500260616
C	6.0	7.2123975353	1.4107391299	1.2799665725
H	1.0	-4.0238908936	-2.5415745489	0.8204201730
H	1.0	6.9227602583	-2.0762096822	1.5838119922
H	1.0	-5.1076394959	1.6184724200	1.5329974745
H	1.0	7.8044415453	2.0893187045	0.6571881607
H	1.0	-4.0011289435	-1.8950398195	2.4720743163
H	1.0	6.9290488875	-0.8600747499	2.8752329052
H	1.0	-4.6920949928	0.5711896564	2.9016022014
H	1.0	7.4584257617	1.6077587954	2.3291417209
H	1.0	-2.7673196913	-1.3876987783	1.3074900002
H	1.0	5.6180635501	-0.8790116532	1.6848831022
H	1.0	-3.4277425768	1.1035721937	1.7877660868
H	1.0	6.1545922427	1.6437736039	1.1307781641
C	6.0	1.3102459014	0.6224383201	-1.7149420637
C	6.0	2.5314327412	0.5768697744	-1.0073984140
C	6.0	1.2374101229	0.2635596841	-3.1843944810
C	6.0	-1.2618023550	0.6505277798	-3.1077436540
C	6.0	3.7546000779	-0.0635269361	-3.1338754451
C	6.0	2.5755914629	0.6002145046	-3.8561528594
C	6.0	0.0486097401	0.9944823019	-3.8235676131
H	1.0	3.7216461924	-1.1505611907	-3.3065920057
H	1.0	4.6918736681	0.2843615021	-3.5834772758

H	1.0	-1.5752194613	-0.3657313869	-3.3872542626
H	1.0	-2.0579983929	1.3196092991	-3.4611311284
H	1.0	1.0667368672	-0.8218568978	-3.2773230467
H	1.0	2.5530169948	0.2801881169	-4.9045485092
H	1.0	2.7106667474	1.6906689335	-3.8554285147
H	1.0	-0.0302390875	0.7307363621	-4.8843248272
H	1.0	0.2318804447	2.0767374562	-3.7736087100
N	7.0	0.2670558015	1.4240197257	0.2968588067
N	7.0	2.5420032907	0.8149348804	0.3567065272
C	6.0	1.4794974261	1.2261139067	0.9736616596
C	6.0	1.5775304997	1.5095432797	2.4476692718
H	1.0	0.8550196005	0.9185128067	3.0155308390
H	1.0	1.3836566017	2.5632451179	2.6737467620
H	1.0	2.5926966369	1.2607230666	2.7587599293
C	6.0	-0.7304154939	2.3351561741	0.8458016677
C	6.0	-1.2021707605	3.4571038020	-0.0536400023
H	1.0	-0.7699613202	3.4343427886	-1.0530112844
H	1.0	-0.9165545051	4.3913697127	0.4443156646
H	1.0	-2.2933998134	3.4426055567	-0.1245302046
O	8.0	-1.0708747352	2.2414242783	2.0049708057

I



E(B3LYP-PCM): S0 = –1884.937592
E(HOMO) = –0.1757; E(LUMO) = –0.1048

E(TDDFT-B3LYP-PCM): S1 = –1884.869149*
Oscillator strength S0 → S1 = 2.6122*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
160	163	0.042927	0.023224
162	163	-1.004526	0.162395
161	164	-0.099333	-0.017325

E(ORMAS-PT2-PCM): S0 = –1880.038827
E(ORMAS-PT2-PCM): S1 = –1879.989968*

Optimized B3LYP-PCM geometry:

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0823837608	0.6016034265	-0.8665030479
C	6.0	-1.1592300048	0.4563513849	-1.5428919476
C	6.0	3.8267066201	0.4767767352	-1.5714013373
C	6.0	-2.3244009808	0.2246009664	-0.8077599448
C	6.0	5.0038340984	0.2657502505	-0.8493453117
H	1.0	-2.2143558767	0.2024257018	0.2680372288
H	1.0	4.9091572866	0.2555657007	0.2280960877
C	6.0	-3.5981908553	-0.0089515799	-1.3535991801
C	6.0	6.2728969561	0.0393345953	-1.4093159982
H	1.0	-3.6949496805	0.0038111800	-2.4335935999
H	1.0	6.3541249805	0.0352673030	-2.4906388879
C	6.0	-4.7538059195	-0.2790531898	-0.6260256139
C	6.0	7.4420445491	-0.2032208243	-0.6938657691
N	7.0	-5.9544679047	-0.4889532638	-1.2364811242
N	7.0	8.6366196749	-0.4083655386	-1.3177772145
C	6.0	-6.1586252023	-0.4341342792	-2.6793121821
C	6.0	8.8203392972	-0.3767709398	-2.7640487001
H	1.0	-7.2197135606	-0.5400560890	-2.8991147783
H	1.0	9.8801820007	-0.4682951467	-2.9957181996
H	1.0	-5.6111501229	-1.2420169942	-3.1762669606
H	1.0	8.2807229046	-1.2029847168	-3.2390075116

H	1.0	-5.8153792926	0.5282332066	-3.0706767905
H	1.0	8.4553347420	0.5722051012	-3.1681686373
C	6.0	-6.9731466745	-0.7681301308	-0.3006878070
C	6.0	9.6722378332	-0.6570044639	-0.3920851990
C	6.0	-8.3205690704	-1.0473533491	-0.5232547982
C	6.0	11.0195657064	-0.9239432601	-0.6296736237
H	1.0	-8.7478742208	-1.0841591326	-1.5197300270
H	1.0	11.4324657397	-0.9744179463	-1.6316128958
C	6.0	-9.1225940336	-1.2858505013	0.6000369200
C	6.0	11.8410191774	-1.1317475059	0.4856230139
H	1.0	-10.1767769428	-1.5066832443	0.4576770515
H	1.0	12.8956342047	-1.3424639711	0.3315134323
C	6.0	-8.5910733611	-1.2455409807	1.8932551099
C	6.0	11.3280294893	-1.0738360150	1.7856548118
H	1.0	-9.2337002756	-1.4331791403	2.7485711409
H	1.0	11.9854208324	-1.2377419660	2.6346037031
C	6.0	-7.2308525599	-0.9657460299	2.0921312398
C	6.0	9.9675860842	-0.8066230000	1.9997249516
H	1.0	-6.8193395407	-0.9374509518	3.0979261856
H	1.0	9.5711165293	-0.7641949660	3.0110785555
C	6.0	-6.4257478813	-0.7293892609	0.9862755789
C	6.0	9.1432710362	-0.6008867370	0.9018922125
C	6.0	-4.9415670710	-0.4106901434	0.8960075180
C	6.0	7.6539749844	-0.3024763382	0.8275915785
C	6.0	-4.1086732226	-1.5803065175	1.4775305604
C	6.0	6.8450472611	-1.4695598394	1.4466203981
C	6.0	-4.6346772564	0.9168945863	1.6324398792
C	6.0	7.3417603137	1.0367841493	1.5402780446
H	1.0	-4.3239876246	-2.5145391319	0.9490176806
H	1.0	7.0627058498	-2.4119477119	0.9337846258
H	1.0	-5.2134222069	1.7440834535	1.2093488435
H	1.0	7.9070038331	1.8608676607	1.0934024420
H	1.0	-4.3627160405	-1.7184405567	2.5338627799
H	1.0	7.1187339981	-1.5826956479	2.5010477264
H	1.0	-4.9009068701	0.8174552223	2.6901453816
H	1.0	7.6212386043	0.9624748910	2.5966699705
H	1.0	-3.0346227019	-1.3868045548	1.4102583095
H	1.0	5.7676916206	-1.2903951905	1.3942782714
H	1.0	-3.5735613248	1.1758260180	1.5752371217
H	1.0	6.2774354463	1.2839437352	1.4897830196
C	6.0	1.3331339917	0.6609629566	-1.5182386897
C	6.0	2.5918960015	0.6144485179	-0.8808482075
C	6.0	1.3237162633	0.6103892151	-3.0497888700
C	6.0	-1.1844159485	0.5237232563	-3.0570463405
C	6.0	3.8318813209	0.5324649448	-3.0861858233
C	6.0	2.5914628366	1.2415386782	-3.6276217669
C	6.0	0.0469399405	1.2395504521	-3.6101394219
H	1.0	3.8848920531	-0.4848955470	-3.5029779009
H	1.0	4.7339518479	1.0518642979	-3.4292247914
H	1.0	-1.2408258760	-0.4907813473	-3.4802639049
H	1.0	-2.0924230838	1.0432740460	-3.3840903885
H	1.0	1.3224610733	-0.4522394521	-3.3466573871

H	1.0	2.5688020171	1.1758627539	-4.7217443332
H	1.0	2.6245170163	2.3079496093	-3.3649021615
H	1.0	0.0566471720	1.1785971986	-4.7047194342
H	1.0	0.0136373953	2.3047112522	-3.3424323333
O	8.0	-0.0275433995	0.5797359883	0.5117719125
O	8.0	2.7188593856	0.5995127415	0.4955934467
C	6.0	0.6477614635	1.5195062433	1.2697908916
C	6.0	2.0388557886	1.5297138910	1.2610497643
C	6.0	-0.0612401897	2.3871757188	2.0966887236
C	6.0	2.7454620108	2.4077681702	2.0789654112
C	6.0	0.6420023868	3.2673775775	2.9241678739
C	6.0	2.0399462517	3.2777033473	2.9152797311
H	1.0	-1.1463997638	2.3589605429	2.0924983800
H	1.0	3.8307754919	2.3952682930	2.0611199588
H	1.0	2.5858385585	3.9619098631	3.5579313733
H	1.0	0.0943608292	3.9435134497	3.5738437704

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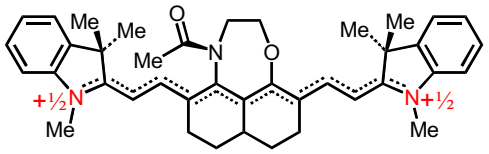

E(B3LYP-PCM): S0 = –1865.314412
E(HOMO) = –0.1751; E(LUMO) = –0.1071

E(TDDFT-B3LYP-PCM): S1 = –1865.247804*
Oscillator strength S0 → S1 = 2.6295*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
159	162	0.044590	0.023541
161	162	-1.006824	0.175205
160	163	0.097073	0.019701
159	166	0.034569	0.012572

E(ORMAS-PT2-PCM): S0 = –1860.448894
E(ORMAS-PT2-PCM): S1 = –1860.400804*

Optimized B3LYP-PCM geometry:

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0903839766	0.2343956470	-0.8708057439
C	6.0	-1.1212332794	-0.0051367150	-1.5725121143
C	6.0	3.8369850427	0.5276912515	-1.4689965662
C	6.0	-2.3160010717	-0.1069332034	-0.8547588957
C	6.0	5.0181065925	0.2284974500	-0.7826389465
H	1.0	-2.2361702597	0.0638669791	0.2110912058
H	1.0	4.9074929965	-0.1184123496	0.2372213672
C	6.0	-3.5789223055	-0.4085033428	-1.3903990995
C	6.0	6.3129489281	0.3046750815	-1.3210602838
H	1.0	-3.6442457190	-0.6027369530	-2.4555825207
H	1.0	6.4163961976	0.6841131130	-2.3318015103
C	6.0	-4.7663584273	-0.4879782547	-0.6672251423
C	6.0	7.4871592124	-0.0699721024	-0.6722930363
N	7.0	-5.9521089918	-0.7937432754	-1.2645794629
N	7.0	8.7060668597	0.0605521821	-1.2660018598
C	6.0	-6.1025752166	-1.0739117504	-2.6879310146
C	6.0	8.9123717857	0.6054565440	-2.6030475417
H	1.0	-7.1462247495	-1.2940759057	-2.9049781471
H	1.0	9.9791254936	0.6454019651	-2.8157641751
H	1.0	-5.4938599421	-1.9386265664	-2.9703190117
H	1.0	8.4259450282	-0.0271282613	-3.3528917743
H	1.0	-5.7948872593	-0.2065869657	-3.2809160418

H	1.0	8.5042525265	1.6189718731	-2.6668338683
C	6.0	-7.0153944849	-0.8032518614	-0.3369439793
C	6.0	9.7439963619	-0.4111605318	-0.4339798971
C	6.0	-8.3670516708	-1.0661090577	-0.5530215230
C	6.0	11.1147476316	-0.4593887978	-0.6812825905
H	1.0	-8.7610849693	-1.3067459703	-1.5347032899
H	1.0	11.5485277089	-0.1112145690	-1.6126279123
C	6.0	-9.2191521056	-1.0095788354	0.5568944158
C	6.0	11.9324300999	-0.9843229719	0.3273596017
H	1.0	-10.2779879899	-1.2101855158	0.4190801316
H	1.0	13.0051863399	-1.0351364309	0.1631959784
C	6.0	-8.7310209937	-0.7018895498	1.8310051648
C	6.0	11.3924955116	-1.4410081919	1.5341693446
H	1.0	-9.4114914424	-0.6651840027	2.6768265328
H	1.0	12.0473472070	-1.8448759232	2.3009232851
C	6.0	-7.3660770510	-0.4404963969	2.0239738610
C	6.0	10.0091628375	-1.3827208381	1.7601024741
H	1.0	-6.9906356404	-0.2020316561	3.0159654725
H	1.0	9.5929951413	-1.7397891990	2.6987392384
C	6.0	-6.5113611767	-0.4918362131	0.9309140128
C	6.0	9.1881888813	-0.8649042282	0.7671030670
C	6.0	-5.0109653215	-0.2600350493	0.8352025867
C	6.0	7.6784450151	-0.6864905280	0.7250358880
C	6.0	-4.2566594462	-1.2937156572	1.7079606103
C	6.0	6.9756756753	-2.0624930492	0.8392824681
C	6.0	-4.6647534266	1.1898320448	1.2558975219
C	6.0	7.2223896767	0.2691002676	1.8557684847
H	1.0	-4.5185252394	-2.3166546674	1.4195025257
H	1.0	7.3099354437	-2.7397814438	0.0469056759
H	1.0	-5.1909468818	1.9156703195	0.6275381214
H	1.0	7.7037009976	1.2477744636	1.7632770083
H	1.0	-4.5323245333	-1.1526426895	2.7585853087
H	1.0	7.2193497253	-2.5182534892	1.8049459240
H	1.0	-4.9706805544	1.3520113057	2.2951650104
H	1.0	7.5008104994	-0.1591524855	2.8246635967
H	1.0	-3.1722925222	-1.1804315727	1.6261671236
H	1.0	5.8882004567	-1.9676749827	0.7741331675
H	1.0	-3.5917747657	1.3879279325	1.1842046747
H	1.0	6.1385864249	0.4151072232	1.8570551418
C	6.0	1.3539605298	0.3372236843	-1.5039186024
C	6.0	2.5813087858	0.4195075041	-0.8077682794
C	6.0	1.4170124113	0.3360495266	-3.0313049784
C	6.0	-1.0656831751	-0.1493872185	-3.0782485194
C	6.0	3.8831540608	0.8907577137	-2.9410320560
C	6.0	2.5189356792	1.3001295635	-3.4943305435
C	6.0	0.0682736886	0.6945792736	-3.6616905840
H	1.0	4.2685612770	0.0309286010	-3.5087669066
H	1.0	4.6057328610	1.7025630643	-3.0987967721
H	1.0	-0.9189970979	-1.2055369832	-3.3511565197
H	1.0	-2.0177368747	0.1561735538	-3.5243668645
H	1.0	1.6904783833	-0.6786089724	-3.3649311824
H	1.0	2.5554957410	1.3252771524	-4.5898611967

H	1.0	2.2631256949	2.3140462927	-3.1575972303
H	1.0	0.1257634026	0.5550824158	-4.7475741678
H	1.0	-0.1441772352	1.7581072117	-3.4835192853
O	8.0	-0.0266710230	0.4300899168	0.4868218853
N	7.0	2.5911823351	0.2557239986	0.6116407115
C	6.0	0.4247203743	-0.6011949401	1.3819463361
C	6.0	1.9006334623	-0.9308396646	1.1295276600
C	6.0	2.9083924311	1.2595724533	1.5127335657
O	8.0	2.8108798582	1.0557920932	2.7229201528
C	6.0	3.3577113450	2.6032875281	0.9689290345
H	1.0	4.3923322098	2.5630270553	0.6145738830
H	1.0	3.2947847329	3.3270174773	1.7834800942
H	1.0	2.7342586284	2.9332922023	0.1327288854
H	1.0	2.3789699843	-1.2525523004	2.0572210550
H	1.0	2.0111225089	-1.7242974521	0.3881885365
H	1.0	0.2822176881	-0.1725928528	2.3747148988
H	1.0	-0.2011076357	-1.4973001901	1.2818993268

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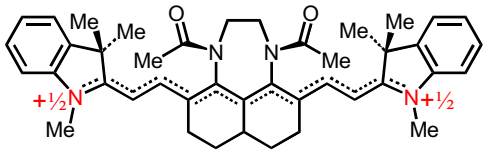


E(B3LYP-PCM): S0 = –1998.027445
E(HOMO) = –0.1767; E(LUMO) = –0.1127

E(TDDFT-B3LYP-PCM): S1 = –1997.963356*
Oscillator strength S0 → S1 = 2.5304*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
170	173	0.040324	0.021788
172	173	1.009972	-0.192903
171	174	0.095521	0.023043
170	177	-0.030110	-0.011673

E(ORMAS-PT2-PCM): S0 = –1992.838947
E(ORMAS-PT2-PCM): S1 = –1992.793110*

Optimized B3LYP-PCM geometry:

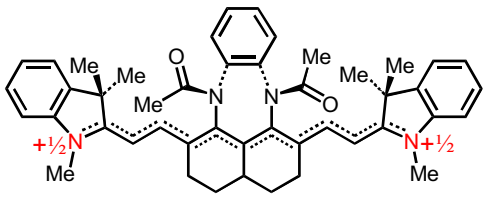
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0903778370	0.5864856729	-0.7526952622
C	6.0	-1.1663470802	0.5757633024	-1.4141412125
C	6.0	3.7950611731	0.2564569745	-1.5442357746
C	6.0	-2.3238416374	0.1832973006	-0.7267158265
C	6.0	4.9994904357	0.1056699996	-0.8454145083
H	1.0	-2.1924676318	-0.1665715532	0.2896518740
H	1.0	4.9523558875	0.2417061928	0.2274945034
C	6.0	-3.6166962434	0.1741964893	-1.2661521072
C	6.0	6.2426173081	-0.2276646423	-1.4026270948
H	1.0	-3.7440105801	0.5566681115	-2.2726531366
H	1.0	6.3011829153	-0.3498701585	-2.4784096384
C	6.0	-4.7666687512	-0.2818455695	-0.6193076751
C	6.0	7.4234944661	-0.4222220263	-0.6868672884
N	7.0	-5.9880355854	-0.2222042489	-1.2122539927
N	7.0	8.6016400645	-0.6943028419	-1.3119383555
C	6.0	-6.2286142675	0.3204411968	-2.5456087697
C	6.0	8.7687644642	-0.7692294984	-2.7594994835
H	1.0	-7.2977780498	0.3174616464	-2.7488839082
H	1.0	9.8302710890	-0.8186484798	-2.9964433216
H	1.0	-5.7216315152	-0.2873009153	-3.3019967006
H	1.0	8.2715647469	-1.6582013781	-3.1621128217
H	1.0	-5.8639412100	1.3502885460	-2.6045447110

H	1.0	8.3491809110	0.1245307540	-3.2292296395
C	6.0	-6.9971275080	-0.7605910471	-0.3837847326
C	6.0	9.6476612427	-0.8989555781	-0.3870571847
C	6.0	-8.3620747692	-0.8882565518	-0.6337227249
C	6.0	10.9836726736	-1.2147349266	-0.6284249921
H	1.0	-8.8145272109	-0.5609127084	-1.5636124056
H	1.0	11.3745101028	-1.3517031590	-1.6310126234
C	6.0	-9.1473467890	-1.4664903625	0.3710582976
C	6.0	11.8211162316	-1.3579372883	0.4846447915
H	1.0	-10.2150676767	-1.5801962778	0.2061687968
H	1.0	12.8675788982	-1.6048348981	0.3291073380
C	6.0	-8.5810910588	-1.8974094993	1.5755573566
C	6.0	11.3333713050	-1.1918362996	1.7852484718
H	1.0	-9.2114180886	-2.3432366260	2.3395259058
H	1.0	12.0027014195	-1.3081345246	2.6326817965
C	6.0	-7.2040705245	-1.7584579981	1.8038205620
C	6.0	9.9835857844	-0.8777145801	2.0028725513
H	1.0	-6.7686667144	-2.0956577304	2.7409552306
H	1.0	9.6083942293	-0.7515831138	3.0152622612
C	6.0	-6.4148421182	-1.1871597853	0.8142769621
C	6.0	9.1431697155	-0.7346275046	0.9070634776
C	6.0	-4.9188569540	-0.9176555968	0.7735442690
C	6.0	7.6599243644	-0.4067022739	0.8347523562
C	6.0	-4.1327609179	-2.2491171272	0.8801367703
C	6.0	6.8357428268	-1.5038793279	1.5528995027
C	6.0	-4.5216910158	0.0563089181	1.9114862469
C	6.0	7.3929107890	0.9882017794	1.4557956156
H	1.0	-4.4266755525	-2.9434943039	0.0865987770
H	1.0	7.0159458383	-2.4873287383	1.1074313839
H	1.0	-5.0470589107	1.0116471908	1.8145651127
H	1.0	7.9401758931	1.7696969859	0.9190846821
H	1.0	-4.3473844861	-2.7202583324	1.8449965696
H	1.0	7.1271095744	-1.5467896122	2.6077454240
H	1.0	-4.7934284272	-0.3868442605	2.8753959555
H	1.0	7.7301551167	0.9907856607	2.4978461861
H	1.0	-3.0533103815	-2.0875682161	0.8133867928
H	1.0	5.7625679671	-1.2981544551	1.5069911895
H	1.0	-3.4456272591	0.2509627136	1.9299379379
H	1.0	6.3295961227	1.2445647198	1.4519114256
C	6.0	1.3231468682	0.5586880278	-1.4575037763
C	6.0	2.5978707774	0.5710916288	-0.8431599340
C	6.0	1.2336830989	0.4500827992	-2.9786749657
C	6.0	-1.2489333626	0.9167699541	-2.8899162587
C	6.0	3.7234125383	0.0367540310	-3.0403570986
C	6.0	2.5577898351	0.8090309007	-3.6554695476
C	6.0	0.0933268285	1.3507919398	-3.4765785266
H	1.0	3.6137125581	-1.0371788876	-3.2544099753
H	1.0	4.6602198234	0.3498787236	-3.5133129646
H	1.0	-1.6220289696	0.0374723190	-3.4348734588
H	1.0	-1.9968594458	1.7060401198	-3.0457603204
H	1.0	0.9859562351	-0.5916175473	-3.2413023088
H	1.0	2.4876059221	0.5996038333	-4.7289644913

H	1.0	2.7411012191	1.8876740668	-3.5498739870
H	1.0	0.0461974807	1.3223410848	-4.5714064269
H	1.0	0.3150106552	2.3883073998	-3.1916510092
N	7.0	0.0939802184	0.4567904253	0.6664749392
N	7.0	2.7188789230	0.8793719411	0.5585022099
C	6.0	0.9030326280	-0.6356330736	1.2273898012
C	6.0	2.3187984363	-0.1327899327	1.5436522394
C	6.0	3.1883359764	2.1005659199	1.0077120238
C	6.0	-0.4436945184	1.3808097484	1.5509611040
O	8.0	3.3860584657	2.3100129486	2.2059448202
O	8.0	-0.4181763687	1.1626458090	2.7620703480
C	6.0	3.4564217449	3.1798607947	-0.0266119397
C	6.0	-1.0356258467	2.6666321486	1.0025556262
H	1.0	4.4435472388	3.0383890575	-0.4802363123
H	1.0	3.4504768015	4.1417797869	0.4895063650
H	1.0	2.7180621135	3.1877449420	-0.8324159108
H	1.0	-0.5678070135	2.9968017901	0.0724035952
H	1.0	-2.1076898572	2.5463223760	0.8134948025
H	1.0	-0.9137561236	3.4330189086	1.7713917211
H	1.0	2.3484695153	0.3620360001	2.5135279469
H	1.0	3.0249963030	-0.9728557723	1.5567410394
H	1.0	0.9177056761	-1.4447907532	0.4947908005
H	1.0	0.4228524666	-1.0009818872	2.1370493977

L



E(B3LYP-PCM): S0 = –2150.354749
E(HOMO) = –0.1769; E(LUMO) = –0.1144

E(TDDFT-B3LYP-PCM): S1 = –2150.291612*
Oscillator strength S0 → S1 = 2.5201*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
182	185	-0.048893	-0.023866
184	185	-1.011258	0.200300
183	186	0.098431	0.026181
182	191	0.030842	0.011708

E(ORMAS-PT2-PCM): S0 = –2144.816388
E(ORMAS-PT2-PCM): S1 = –2144.773498*

Optimized B3LYP-PCM geometry:

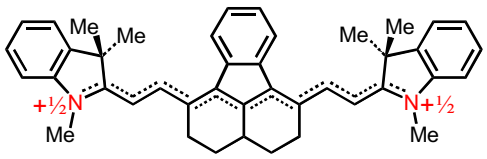
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0512625228	0.2930629867	-0.7424893875
C	6.0	-1.1694294561	0.1172154424	-1.4440939037
C	6.0	3.8158676214	0.4348325731	-1.4175050268
C	6.0	-2.3715227222	-0.0936503672	-0.7525669178
C	6.0	5.0127760127	0.1493350746	-0.7436794632
H	1.0	-2.3183062682	-0.0962134601	0.3271042475
H	1.0	4.9384862713	-0.1027990800	0.3059075569
C	6.0	-3.6214725358	-0.3158062837	-1.3457586347
C	6.0	6.2849860606	0.1365633181	-1.3332091162
H	1.0	-3.6667723884	-0.3657734247	-2.4275031727
H	1.0	6.3569215847	0.4072275717	-2.3800873233
C	6.0	-4.8322860956	-0.4686069326	-0.6680811526
C	6.0	7.4836439645	-0.1834448391	-0.6938472958
N	7.0	-5.9947538455	-0.7087617018	-1.3309251179
N	7.0	8.6741267596	-0.1298888965	-1.3485248029
C	6.0	-6.0997971737	-0.8596644077	-2.7789519391
C	6.0	8.8252009796	0.2642097211	-2.7460194491
H	1.0	-7.1198471373	-1.1355949119	-3.0395621618
H	1.0	9.8804068521	0.2549937965	-3.0118111281
H	1.0	-5.4244684776	-1.6479105708	-3.1239822642

H	1.0	8.2898059290	-0.4335070062	-3.3974659193
H	1.0	-5.8473834012	0.0799945256	-3.2812172656
H	1.0	8.4327997627	1.2745304618	-2.8964052720
C	6.0	-7.0927068705	-0.7881741774	-0.4465281951
C	6.0	9.7485014078	-0.4950639348	-0.5087783255
C	6.0	-8.4377776197	-1.0126945828	-0.7343410178
C	6.0	11.1085699123	-0.5654222580	-0.8044570924
H	1.0	-8.7987749454	-1.1537712543	-1.7474753186
H	1.0	11.5017121778	-0.3275968614	-1.7870376886
C	6.0	-9.3279618680	-1.0492934563	0.3457873975
C	6.0	11.9699555634	-0.9606929855	0.2261151247
H	1.0	-10.3831068236	-1.2225848815	0.1539016821
H	1.0	13.0359341484	-1.0249300228	0.0266522291
C	6.0	-8.8824031614	-0.8666199142	1.6594071700
C	6.0	11.4818502378	-1.2723800278	1.4995728697
H	1.0	-9.5930054721	-0.8990842817	2.4801773325
H	1.0	12.1704936193	-1.5769533311	2.2823385172
C	6.0	-7.5236637651	-0.6405189259	1.9240057354
C	6.0	10.1081691385	-1.1951904363	1.7729491733
H	1.0	-7.1816670115	-0.4981783202	2.9459120650
H	1.0	9.7335029369	-1.4398596021	2.7635516827
C	6.0	-6.6314817138	-0.6014238669	0.8608062574
C	6.0	9.2439885235	-0.8038687077	0.7589280954
C	6.0	-5.1278916794	-0.3777338587	0.8384839195
C	6.0	7.7319365010	-0.6393342219	0.7544661490
C	6.0	-4.4144906608	-1.4950478050	1.6391262989
C	6.0	7.0477833918	-1.9993730913	1.0397795803
C	6.0	-4.7861759053	1.0258268788	1.3998922272
C	6.0	7.3068997154	0.4319517670	1.7899900882
H	1.0	-4.6232573337	-2.4813129251	1.2130678672
H	1.0	7.3807095320	-2.7637542768	0.3305697899
H	1.0	-5.3320949376	1.8055465568	0.8590218009
H	1.0	7.7338176464	1.4091072176	1.5427486242
H	1.0	-4.7703838814	-1.4854361071	2.6745368483
H	1.0	7.3036195899	-2.3334129021	2.0508251618
H	1.0	-5.0757931971	1.0747618048	2.4549360440
H	1.0	7.6700069964	0.1416507680	2.7812524514
H	1.0	-3.3306060324	-1.3522788148	1.6578947724
H	1.0	5.9589795392	-1.9238388431	0.9695307984
H	1.0	-3.7176232361	1.2474916674	1.3260965485
H	1.0	6.2198103767	0.5362198119	1.8540842334
C	6.0	1.3150773380	0.3944021349	-1.3818002918
C	6.0	2.5728281141	0.4413341394	-0.7231697639
C	6.0	1.3441393124	0.3918192236	-2.9136619941
C	6.0	-1.1654953305	0.1433034775	-2.9581008545
C	6.0	3.8471403055	0.6874642025	-2.9106483450
C	6.0	2.5208784162	1.2251553561	-3.4308306623
C	6.0	0.0318283643	0.9118251975	-3.5020008769
H	1.0	4.1002746617	-0.2477081411	-3.4319814688
H	1.0	4.6515532491	1.3949160376	-3.1477578824
H	1.0	-1.1547824346	-0.8868273806	-3.3462060779
H	1.0	-2.0895429320	0.6005972511	-3.3276259411

H	1.0	1.4849368147	-0.6476604553	-3.2539139250
H	1.0	2.5202796369	1.2237635090	-4.5269389032
H	1.0	2.3860039432	2.2677422667	-3.1109147227
H	1.0	0.0667405703	0.8332773648	-4.5948027682
H	1.0	-0.0746642988	1.9778292358	-3.2583720590
N	7.0	-0.0180281831	0.2815602845	0.7021758217
N	7.0	2.6542445230	0.4186528107	0.7144885952
C	6.0	0.6771664278	-0.7884095987	1.3598537647
C	6.0	2.0715490588	-0.7082300255	1.3864339259
C	6.0	0.0235934232	-1.8822053154	1.9291464296
C	6.0	2.8231671613	-1.6983564630	2.0169385979
C	6.0	0.7744756535	-2.8763610336	2.5607074522
C	6.0	2.1683935607	-2.7807996461	2.6099374493
H	1.0	-1.0584861815	-1.9532768662	1.8804264309
H	1.0	3.9045525506	-1.6215850576	2.0523756743
H	1.0	2.7498754467	-3.5545045200	3.1025371203
H	1.0	0.2707463409	-3.7266558665	3.0108442667
C	6.0	3.1367995828	1.4749202658	1.4848683182
C	6.0	-0.4819567703	1.4015348605	1.3900273310
O	8.0	3.2187083281	1.3638167827	2.7059606571
O	8.0	-0.9502491338	2.3648840434	0.7924242437
C	6.0	3.5289932478	2.7574120239	0.7770530999
C	6.0	-0.3873623026	1.3552139240	2.9042000776
H	1.0	4.5801222449	2.7201276527	0.4719267313
H	1.0	3.4110759312	3.5733699292	1.4931674035
H	1.0	2.9276238608	2.9534813078	-0.1135176868
H	1.0	0.6563319936	1.2899180373	3.2300035129
H	1.0	-0.8316788379	2.2720496146	3.2948775847
H	1.0	-0.9150910059	0.4909367294	3.3196851675

M



E(B3LYP-PCM): S0 = –1734.577815
E(HOMO) = –0.1719; E(LUMO) = –0.1171

E(TDDFT-B3LYP-PCM): S1 = –1734.523229*
Oscillator strength S0 → S1 = 1.6629*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
151	155	0.090316	0.031047
152	155	0.147101	0.002842
154	155	1.003265	-0.221991
153	156	0.080972	0.031147
152	157	-0.060973	-0.014437
154	161	-0.030468	-0.016387

E(ORMAS-PT2-PCM): S0 = –1730.007377
E(ORMAS-PT2-PCM): S1 = –1729.963356*

Optimized B3LYP-PCM geometry:

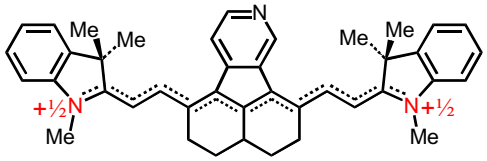
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1068541726	1.1428885274	-1.2163892525
C	6.0	-1.1366570716	0.6539222935	-1.6799540044
C	6.0	3.7002515614	1.3676038683	-1.8665771542
C	6.0	-2.2281993836	0.4499452155	-0.8274553274
C	6.0	4.8666772929	1.5228051847	-1.1074037718
H	1.0	-2.0828709636	0.6835059449	0.2180650965
H	1.0	4.7417279819	1.7467134815	-0.0574712462
C	6.0	-3.4621825895	-0.0999419064	-1.2125791450
C	6.0	6.1742790553	1.3440312388	-1.5887796440
H	1.0	-3.5929679841	-0.3439739792	-2.2606763862
H	1.0	6.2891954884	1.0997199101	-2.6384973867
C	6.0	-4.5377971252	-0.3861915696	-0.3742234826
C	6.0	7.3485416710	1.4333713960	-0.8431665106
N	7.0	-5.6908476157	-0.9298728819	-0.8556762967
N	7.0	8.5698980211	1.2206690299	-1.4081003328
C	6.0	-5.9250513757	-1.2481957252	-2.2596883502
C	6.0	8.7758280336	0.8769111596	-2.8110524497
H	1.0	-6.9478468621	-1.5989893658	-2.3845540011
H	1.0	9.8361109168	0.7078776891	-2.9893102475
H	1.0	-5.2379733774	-2.0323001753	-2.5946660198

H	1.0	8.2276880849	-0.0372412960	-3.0583684267
H	1.0	-5.7844159838	-0.3563077547	-2.8777623977
H	1.0	8.4327012846	1.6909384086	-3.4576554272
C	6.0	-6.6243371251	-1.1674483801	0.1744806092
C	6.0	9.6112707869	1.3683024212	-0.4681314987
C	6.0	-7.8994208919	-1.7245741745	0.0924220405
C	6.0	10.9869900000	1.2408435924	-0.6537252200
H	1.0	-8.3286622317	-2.0545360851	-0.8475577714
H	1.0	11.4221174255	0.9978249130	-1.6171966145
C	6.0	-8.6234491631	-1.8521006653	1.2841161823
C	6.0	11.8076388626	1.4421302554	0.4627722938
H	1.0	-9.6193830142	-2.2847258826	1.2515624055
H	1.0	12.8840724542	1.3495993640	0.3489665233
C	6.0	-8.0861433787	-1.4363004492	2.5069632560
C	6.0	11.2663647169	1.7582226634	1.7133891483
H	1.0	-8.6671655511	-1.5457278724	3.4180920935
H	1.0	11.9238196180	1.9093917162	2.5646161998
C	6.0	-6.8003105732	-0.8783860730	2.5648233177
C	6.0	9.8784177329	1.8828297406	1.8755623804
H	1.0	-6.3854586068	-0.5579384281	3.5171154825
H	1.0	9.4615237951	2.1298480182	2.8485531481
C	6.0	-6.0719601269	-0.7483035208	1.3897643308
C	6.0	9.0542473727	1.6863717526	0.7756196750
C	6.0	-4.6780016246	-0.1903091269	1.1451528923
C	6.0	7.5409153315	1.7610426540	0.6470322768
C	6.0	-3.6261429524	-1.0040365629	1.9382484749
C	6.0	6.8710606840	0.7066874633	1.5629673119
C	6.0	-4.6325708860	1.3099095530	1.5279673351
C	6.0	7.0484057206	3.1905768456	0.9843904280
H	1.0	-3.6299595935	-2.0552995862	1.6330518335
H	1.0	7.2098669040	-0.3035350611	1.3122490473
H	1.0	-5.3823524678	1.8806746014	0.9709918856
H	1.0	7.5293360675	3.9343921595	0.3412649021
H	1.0	-3.8598328288	-0.9570462875	3.0071208365
H	1.0	7.1380715817	0.9091339125	2.6056213715
H	1.0	-4.8414139197	1.4207132968	2.5972836025
H	1.0	7.2937526384	3.4260450732	2.0252432625
H	1.0	-2.6156880404	-0.6099985626	1.7987425756
H	1.0	5.7807786786	0.7319855278	1.4831041189
H	1.0	-3.6510041875	1.7491812299	1.3279924133
H	1.0	5.9656164050	3.2844210853	0.8630741499
C	6.0	1.2696717423	1.0356108754	-2.0015372322
C	6.0	2.4075747300	1.4843498832	-1.3049806897
C	6.0	1.2930568437	0.4933250249	-3.3961310969
C	6.0	-1.2178041666	0.2315106314	-3.1462890341
C	6.0	3.7890314580	0.9423574661	-3.3315238137
C	6.0	2.4856604821	1.1254197404	-4.1285777997
C	6.0	-0.0786830335	0.7707992585	-4.0284932603
H	1.0	4.0968071593	-0.1137267186	-3.3766292084
H	1.0	4.5868331192	1.5083282226	-3.8271675895
H	1.0	-1.2300891802	-0.8680192657	-3.2001449715
H	1.0	-2.1756144558	0.5617162252	-3.5665334036

H	1.0	1.4462812563	-0.5995092736	-3.3690419219
H	1.0	2.6047642642	0.6865124473	-5.1262530046
H	1.0	2.2894144415	2.1977136540	-4.2667891768
H	1.0	-0.1461885121	0.3204620886	-5.0260226866
H	1.0	-0.1956613756	1.8561003146	-4.1548099362
C	6.0	1.9253582991	2.0030285874	0.0066732679
C	6.0	0.5142611992	1.7925262302	0.0605680739
C	6.0	2.5622001903	2.6870052348	1.0370753090
C	6.0	1.8169579683	3.1331988071	2.1431684463
C	6.0	-0.2185755405	2.2738498693	1.1401921744
C	6.0	0.4423969060	2.9294397120	2.1941302646
H	1.0	2.3214127471	3.6582446772	2.9495506137
H	1.0	3.6197484089	2.9205807841	0.9983098414
H	1.0	-0.1331211649	3.2938005368	3.0404686351
H	1.0	-1.2984183010	2.1894407423	1.1790609236

N



E(B3LYP-PCM): S0 = –1750.615134
E(HOMO) = –0.1740; E(LUMO) = –0.1212

E(TDDFT-B3LYP-PCM): S1 = –1750.561122*
Oscillator strength S0 → S1 = 1.7771*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
148	155	0.050759	0.014527
151	155	-0.077667	-0.023384
152	155	-0.060865	0.009652
154	155	-1.014672	0.238269
153	156	0.084008	0.033744
152	157	-0.059195	-0.018200
154	157	-0.035088	-0.008509
154	161	-0.032030	-0.018408

E(ORMAS-PT2-PCM): S0 = –1746.035984
E(ORMAS-PT2-PCM): S1 = –1745.992392*

Optimized B3LYP-PCM geometry:

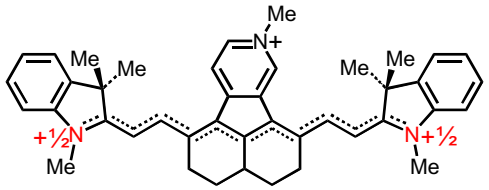
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1199947013	1.0460761015	-1.1935505541
C	6.0	-1.1320125206	0.5864565048	-1.6647687089
C	6.0	3.7111056002	1.3165396979	-1.8566867813
C	6.0	-2.2322225948	0.4013060225	-0.8194636594
C	6.0	4.8818665116	1.4948770423	-1.1043691619
H	1.0	-2.0913954180	0.6327459061	0.2269687034
H	1.0	4.7596223894	1.7173901949	-0.0538493106
C	6.0	-3.4739017252	-0.1232316958	-1.2131450315
C	6.0	6.1863960266	1.3440742394	-1.5942275186
H	1.0	-3.6006377226	-0.3708284880	-2.2608241009
H	1.0	6.3006740766	1.1002052975	-2.6439931313
C	6.0	-4.5628925969	-0.3817835749	-0.3821985219
C	6.0	7.3645999659	1.4592205410	-0.8532496406
N	7.0	-5.7210623537	-0.9070675670	-0.8698688541
N	7.0	8.5840921121	1.2696662516	-1.4237682664
C	6.0	-5.9471932164	-1.2356361163	-2.2731296248
C	6.0	8.7909903285	0.9253739705	-2.8274655912

H	1.0	-6.9714231630	-1.5802542320	-2.4026563049
H	1.0	9.8525982960	0.7670145421	-3.0068181190
H	1.0	-5.2636056745	-2.0279231951	-2.5953663163
H	1.0	8.2523060308	0.0048912972	-3.0706880904
H	1.0	-5.7949042186	-0.3502561535	-2.8978050132
H	1.0	8.4380520754	1.7348310692	-3.4741845746
C	6.0	-6.6710254889	-1.1116409430	0.1524122931
C	6.0	9.6286238544	1.4406135892	-0.4898402566
C	6.0	-7.9571043670	-1.6414526939	0.0620868342
C	6.0	11.0052572756	1.3389662257	-0.6835913998
H	1.0	-8.3833743634	-1.9724092545	-0.8788652563
H	1.0	11.4395785212	1.1023477856	-1.6489398205
C	6.0	-8.6967287210	-1.7390015542	1.2468869081
C	6.0	11.8275457805	1.5581504293	0.4280140634
H	1.0	-9.7016911877	-2.1495933624	1.2081878871
H	1.0	12.9048945651	1.4858541486	0.3090751615
C	6.0	-8.1636066152	-1.3208469659	2.4708930662
C	6.0	11.2865432563	1.8667071242	1.6808856943
H	1.0	-8.7569739676	-1.4070576056	3.3765366650
H	1.0	11.9456479114	2.0320760900	2.5281557300
C	6.0	-6.8664988207	-0.7909429933	2.5371596846
C	6.0	9.8976712966	1.9653781774	1.8509231401
H	1.0	-6.4552898390	-0.4685299041	3.4903489698
H	1.0	9.4816961593	2.2064396629	2.8257139513
C	6.0	-6.1226722863	-0.6904060369	1.3688643878
C	6.0	9.0717419172	1.7508343366	0.7556178217
C	6.0	-4.7143901914	-0.1655553223	1.1330717625
C	6.0	7.5570125475	1.7938867312	0.6347817775
C	6.0	-3.6891368288	-0.9924874122	1.9471883360
C	6.0	6.9146556182	0.7264097913	1.5556377027
C	6.0	-4.6409186965	1.3381047732	1.4972498258
C	6.0	7.0352437156	3.2133623543	0.9718075008
H	1.0	-3.7079601885	-2.0457068114	1.6497074238
H	1.0	7.2717946371	-0.2769982658	1.3031828498
H	1.0	-5.3769700610	1.9161603907	0.9295598570
H	1.0	7.4977498471	3.9663741699	0.3259638703
H	1.0	-3.9373207821	-0.9327645196	3.0120844627
H	1.0	7.1849571331	0.9352518383	2.5960694883
H	1.0	-4.8518053725	1.4675622067	2.5640908329
H	1.0	7.2801217716	3.4546195040	2.0113304047
H	1.0	-2.6693964024	-0.6185826414	1.8199122121
H	1.0	5.8235937001	0.7295369372	1.4834588973
H	1.0	-3.6504059852	1.7563511615	1.2951363213
H	1.0	5.9502395488	3.2838725707	0.8548756096
C	6.0	1.2806793277	0.9603400628	-1.9814775546
C	6.0	2.4243481730	1.4005306887	-1.2833214563
C	6.0	1.2988645484	0.4556572749	-3.3901311960
C	6.0	-1.2128405353	0.1862420654	-3.1365914982
C	6.0	3.7944563330	0.9099220034	-3.3261664582
C	6.0	2.4870443666	1.1062426777	-4.1134421997
C	6.0	-0.0762403779	0.7444899014	-4.0107649004
H	1.0	4.1005758881	-0.1459005905	-3.3851430646

H	1.0	4.5902345291	1.4814720623	-3.8179590265
H	1.0	-1.2198036795	-0.9123912306	-3.2068872626
H	1.0	-2.1717190820	0.5188437283	-3.5515437302
H	1.0	1.4543674389	-0.6369336164	-3.3873363961
H	1.0	2.6023815435	0.6887257142	-5.1204684295
H	1.0	2.2885987366	2.1808731072	-4.2281519829
H	1.0	-0.1457349569	0.3139801965	-5.0166456214
H	1.0	-0.1951581457	1.8318117622	-4.1152127702
C	6.0	1.9454608227	1.8718356226	0.0427600566
C	6.0	0.5373469562	1.6538316792	0.0991023699
C	6.0	2.5589049562	2.5188743818	1.1083163491
N	7.0	1.8941407458	2.9131259436	2.2153046236
C	6.0	-0.1543682732	2.0894417143	1.2215362776
C	6.0	0.5785938870	2.6950228719	2.2560117348
H	1.0	3.6153519200	2.7695080665	1.0992162845
H	1.0	0.0615208691	3.0292003842	3.1540346024
H	1.0	-1.2295347128	2.0102533899	1.3249213214

O



E(B3LYP-PCM): S0 = –1790.348664
E(HOMO) = –0.1806; E(LUMO) = –0.1356

E(TDDFT-B3LYP-PCM): S1 = –1790.301813*
Oscillator strength S0 → S1 = 1.3303*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
152	159	0.071530	0.019203
153	159	0.033905	0.009174
158	159	1.021612	-0.274519
156	160	0.043687	0.013357
158	160	0.119880	0.027560
157	161	-0.071513	-0.035950
156	162	0.033898	0.013291
158	162	0.031914	0.010000

E(ORMAS-PT2-PCM): S0 = –1785.649050
E(ORMAS-PT2-PCM): S1 = –1785.607932*

Optimized B3LYP-PCM geometry:

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1052539761	1.0983308864	-1.1932879429
C	6.0	-1.1443833535	0.6195614135	-1.6546526249
C	6.0	3.7109890251	1.3477318988	-1.8322257247
C	6.0	-2.2446644436	0.4298821071	-0.8070902318
C	6.0	4.8826794392	1.5232045930	-1.0739382788
H	1.0	-2.1083431983	0.6592459897	0.2409473816
H	1.0	4.7649296044	1.7515428049	-0.0232208763
C	6.0	-3.4780123729	-0.1034164282	-1.2047829222
C	6.0	6.1801197802	1.3509106318	-1.5654518713
H	1.0	-3.6019084780	-0.3431255695	-2.2543911080
H	1.0	6.2855050421	1.1019181319	-2.6145913622
C	6.0	-4.5680061667	-0.3822248245	-0.3758480131
C	6.0	7.3701839193	1.4483259480	-0.8326890418
N	7.0	-5.7184794160	-0.9067513369	-0.8729200160
N	7.0	8.5765429446	1.2412740914	-1.4150987098
C	6.0	-5.9451781877	-1.2110071697	-2.2830870805

C	6.0	8.7675413584	0.8977146726	-2.8229639960
H	1.0	-6.9712730412	-1.5472072472	-2.4180984984
H	1.0	9.8256563053	0.7283395588	-3.0109705188
H	1.0	-5.2655738571	-2.0019271312	-2.6159077380
H	1.0	8.2168222327	-0.0162032101	-3.0622715994
H	1.0	-5.7873711863	-0.3155784325	-2.8909196134
H	1.0	8.4185778135	1.7140676241	-3.4623876863
C	6.0	-6.6672666104	-1.1406690839	0.1454364997
C	6.0	9.6345328731	1.3951759221	-0.4917566903
C	6.0	-7.9485956813	-1.6801872201	0.0438672679
C	6.0	11.0071763744	1.2727557721	-0.7015340548
H	1.0	-8.3721266285	-1.9968090788	-0.9031006213
H	1.0	11.4277072321	1.0306285164	-1.6714417151
C	6.0	-8.6861683731	-1.8067663903	1.2265900119
C	6.0	11.8432367000	1.4785863205	0.4015259218
H	1.0	-9.6873763323	-2.2254017284	1.1809111864
H	1.0	12.9180640439	1.3905538038	0.2722893015
C	6.0	-8.1557218987	-1.4068443540	2.4583237218
C	6.0	11.3190271592	1.7940222792	1.6604347568
H	1.0	-8.7481602459	-1.5151426466	3.3621068574
H	1.0	11.9896491899	1.9486110590	2.5005810483
C	6.0	-6.8635810309	-0.8672241336	2.5356446805
C	6.0	9.9342262754	1.9133855878	1.8464937426
H	1.0	-6.4552606191	-0.5598292083	3.4948559961
H	1.0	9.5327393545	2.1592901154	2.8259665814
C	6.0	-6.1213979700	-0.7385532912	1.3691301752
C	6.0	9.0944605625	1.7120020261	0.7592611988
C	6.0	-4.7179918564	-0.1993086313	1.1427329322
C	6.0	7.5805356635	1.7761272182	0.6523117329
C	6.0	-3.6852262107	-1.0399732129	1.9335067833
C	6.0	6.9315800886	0.7124546421	1.5731661575
C	6.0	-4.6538823604	1.2957421457	1.5430728331
C	6.0	7.0817835704	3.2023365724	0.9942790535
H	1.0	-3.7066513990	-2.0878520648	1.6182265944
H	1.0	7.2847606053	-0.2924322029	1.3216734375
H	1.0	-5.3888374718	1.8846356413	0.9855464721
H	1.0	7.5581127669	3.9508861351	0.3536962874
H	1.0	-3.9241904080	-0.9980179724	3.0012027644
H	1.0	7.2011705681	0.9213695750	2.6135495824
H	1.0	-4.8715014520	1.3959183428	2.6114157921
H	1.0	7.3242125615	3.4346686103	2.0361231896
H	1.0	-2.6669878278	-0.6635511818	1.8028729022
H	1.0	5.8409071225	0.7192527172	1.4982894803
H	1.0	-3.6640485714	1.7233312935	1.3588787614
H	1.0	5.9989884193	3.2913007846	0.8700614807
C	6.0	1.2781330344	0.9899045894	-1.9664476117
C	6.0	2.4181171206	1.4527202323	-1.2791998673
C	6.0	1.3036278342	0.4502234471	-3.3595971068
C	6.0	-1.2141289922	0.1936805039	-3.1185626109
C	6.0	3.8005433878	0.9105237530	-3.2915852035
C	6.0	2.4974603871	1.0817863967	-4.0913636593
C	6.0	-0.0680849421	0.7281561013	-3.9950276657

H	1.0	4.1133612623	-0.1442600748	-3.3234318650
H	1.0	4.5951708886	1.4759857871	-3.7914508223
H	1.0	-1.2288323013	-0.9057959016	-3.1658806236
H	1.0	-2.1673822899	0.5248100338	-3.5470396076
H	1.0	1.4559330934	-0.6417294321	-3.3229055699
H	1.0	2.6206152055	0.6336863131	-5.0836614591
H	1.0	2.2980542708	2.1516239169	-4.2402546355
H	1.0	-0.1307212600	0.2734755714	-4.9901340410
H	1.0	-0.1825434311	1.8125764681	-4.1271854954
C	6.0	1.9207121939	1.9733126380	0.0135778226
C	6.0	0.5046122784	1.7567630674	0.0599511510
C	6.0	2.5268998084	2.6684595289	1.0355005448
N	7.0	1.7943490022	3.1124933480	2.0988179364
C	6.0	-0.2153887312	2.2532275961	1.1441630123
C	6.0	0.4616386845	2.9147316872	2.1593381236
H	1.0	3.5729767360	2.9368675945	1.0603272348
H	1.0	-0.0442453539	3.3092747155	3.0309995240
H	1.0	-1.2908990817	2.1807259632	1.2257732445
C	6.0	2.4914640625	3.8043141824	3.2059031719
H	1.0	3.1931732403	4.5279089043	2.7890481563
H	1.0	3.0242609303	3.0677068494	3.8114423079
H	1.0	1.7542326089	4.3235422178	3.8164111935

2. Data at singlet excited state optimized geometries: B3LYP-PCM & TDDFT-B3LYP-PCM energies (hartree) & wave function data, ORMAS-PT2-PCM energies (hartree), and TDDFT-B3LYP-PCM optimized geometries (Å)

A

E(B3LYP-PCM): S0 = –1310.841524*
E(HOMO) = –0.1772; E(LUMO) = –0.1093

E(TDDFT-B3LYP-PCM): S1 = –1310.784404
Oscillator strength S1 → S0 = 3.2752*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
117	118	0.998095	-0.095616
116	119	0.096347	0.028598
115	122	0.032597	0.013987

E(ORMAS-PT2-PCM): S0 = –1307.327824*
E(ORMAS-PT2-PCM): S1 = –1307.280219

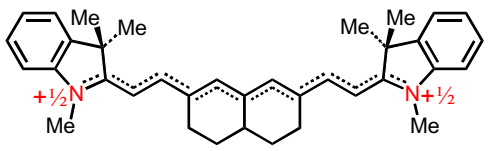
Optimized TDDFT-B3LYP-PCM geometry:

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1094199878	-0.0891771230	-0.3838752050
C	6.0	-1.1318478670	-0.0949150566	-1.0369604707
C	6.0	3.8171617251	-0.0662485128	-1.0665218481
C	6.0	-2.3625543712	-0.1041890027	-0.3762651664
C	6.0	5.0553491958	-0.0567972800	-0.4200087122
H	1.0	-2.3424381413	-0.1074684000	0.7100617770
H	1.0	5.0469453517	-0.0552259242	0.6664548867
C	6.0	-3.5974287700	-0.1093256707	-1.0518834493
C	6.0	6.2825882771	-0.0482460011	-1.1093657282
H	1.0	-3.5468116867	-0.1039898373	-2.1382562697
H	1.0	6.2198917253	-0.0511828651	-2.1951319823
C	6.0	-4.8663503966	-0.1209344097	-0.4810288789
C	6.0	7.5575686640	-0.0365220788	-0.5522123390
N	7.0	-6.0044006098	-0.1241251616	-1.2503297884
N	7.0	8.6876763686	-0.0244961330	-1.3330632606
C	6.0	-6.0041047741	-0.1139753447	-2.7076824951
C	6.0	8.6722148774	-0.0181276753	-2.7903370471
H	1.0	-7.0298211402	-0.1149305505	-3.0720300095
H	1.0	9.6931155874	0.0272215207	-3.1653676487

H	1.0	-5.4920108888	-1.0017373829	-3.0937484213
H	1.0	8.1958153606	-0.9282724036	-3.1704020659
H	1.0	-5.4985566154	0.7829698382	-3.0808111945
H	1.0	8.1237043006	0.8548997428	-3.1587997305
C	6.0	-7.1586214668	-0.1386860947	-0.4616707149
C	6.0	9.8499574058	-0.0206117891	-0.5561540115
C	6.0	-8.4999743092	-0.1472458690	-0.8586772880
C	6.0	11.1873043858	-0.0137411052	-0.9663897945
H	1.0	-8.7927737313	-0.1430817712	-1.9030281872
H	1.0	11.4698053580	-0.0124503973	-2.0136173686
C	6.0	-9.4687474308	-0.1619545266	0.1483875723
C	6.0	12.1660899751	-0.0099780401	0.0311045111
H	1.0	-10.5189624219	-0.1689391571	-0.1295002042
H	1.0	13.2134939120	-0.0047087882	-0.2571062734
C	6.0	-9.1107103276	-0.1679631646	1.5032025131
C	6.0	11.8215313328	-0.0133337527	1.3894694192
H	1.0	-9.8838905537	-0.1794384432	2.2659342669
H	1.0	12.6022031361	-0.0102628604	2.1446071901
C	6.0	-7.7589703691	-0.1592299188	1.8811218521
C	6.0	10.4736787711	-0.0213500272	1.7806515252
H	1.0	-7.4860171204	-0.1640699926	2.9332275108
H	1.0	10.2111377083	-0.0245121860	2.8354404127
C	6.0	-6.7852497553	-0.1446280029	0.8933156240
C	6.0	9.4902495617	-0.0254528975	0.8025412514
C	6.0	-5.2693594471	-0.1330159100	0.9995962909
C	6.0	7.9755067462	-0.0349802673	0.9242102278
C	6.0	-4.7686732682	-1.4097736324	1.7229294661
C	6.0	7.5007543021	-1.3144724225	1.6600808836
C	6.0	-4.7891685288	1.1430106461	1.7380985880
C	6.0	7.4847766140	1.2384612579	1.6604367768
H	1.0	-5.1041803467	-2.3125414013	1.2026235262
H	1.0	7.8427847803	-2.2154480344	1.1409385355
H	1.0	-5.1375283700	2.0463933135	1.2273801309
H	1.0	7.8170736762	2.1437498813	1.1424656155
H	1.0	-5.1672807198	-1.4333623781	2.7430006153
H	1.0	7.9110796197	-1.3270225701	2.6756989076
H	1.0	-5.1896291203	1.1492962055	2.7577132937
H	1.0	7.8934422743	1.2549002995	2.6766638516
H	1.0	-3.6771166511	-1.4341321655	1.7850286371
H	1.0	6.4104251767	-1.3535703490	1.7350115768
H	1.0	-3.6981910429	1.1829777890	1.8024252502
H	1.0	6.3939170643	1.2648570087	1.7334829111
H	1.0	0.1139216266	-0.0910434656	0.7066652180
H	1.0	-1.1351510722	-0.0921904914	-2.1278056600
H	1.0	3.8082301921	-0.0670109874	-2.1573376663
C	6.0	1.3426304632	-0.0811299545	-1.0463616985
C	6.0	2.5836883069	-0.0740702888	-0.3987673742
H	1.0	2.5917063593	-0.0741666811	0.6917527594
H	1.0	1.3363199843	-0.0801355461	-2.1372324019

B



E(B3LYP-PCM): S0 = –1504.877463*
E(HOMO) = –0.1715; E(LUMO) = –0.1055

E(TDDFT-B3LYP-PCM): S1 = –1504.821540
Oscillator strength S1 → S0 = 3.0305*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
133	136	0.038340	0.023236
135	136	-0.998887	0.104123
134	137	0.094350	0.030026
133	140	0.033942	0.014638

E(ORMAS-PT2-PCM): S0 = –1500.848326*
E(ORMAS-PT2-PCM): S1 = –1500.800165

Optimized TDDFT-B3LYP-PCM geometry:

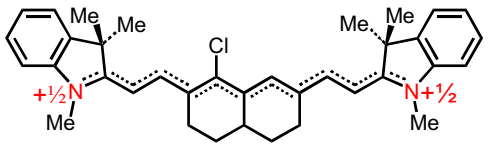
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1197614894	0.0730502497	-1.0188616941
C	6.0	-1.1468212266	0.0432052044	-1.6334111039
C	6.0	3.8255356155	0.0765769119	-1.6625671173
C	6.0	-2.2962160261	-0.0096708628	-0.8229329995
C	6.0	4.9848185804	0.0436027027	-0.8654577617
H	1.0	-2.1115296338	-0.0137753509	0.2474226457
H	1.0	4.8122700342	0.0430622981	0.2068806786
C	6.0	-3.6243681714	-0.0686437770	-1.2760811322
C	6.0	6.3085036439	-0.0006474111	-1.3334175867
H	1.0	-3.7819189993	-0.0747811601	-2.3503679080
H	1.0	6.4539609519	-0.0118129559	-2.4093488094
C	6.0	-4.7702073660	-0.1243697352	-0.4844636845
C	6.0	7.4632747109	-0.0369151568	-0.5538323254
N	7.0	-6.0269076100	-0.1743184260	-1.0363472165
N	7.0	8.7148453186	-0.0759492623	-1.1181870952
C	6.0	-6.2877778729	-0.1751185573	-2.4700882427
C	6.0	8.9604487776	-0.0835240515	-2.5544846638
H	1.0	-7.3616646143	-0.2057938435	-2.6457328761
H	1.0	10.0327420634	-0.1015632528	-2.7415668801
H	1.0	-5.8278330783	-1.0514971681	-2.9389886484
H	1.0	8.5068888663	-0.9690896345	-3.0122344581
H	1.0	-5.8808334722	0.7319344212	-2.9290953538

H	1.0	8.5370837592	0.8151247426	-3.0151961822
C	6.0	-7.0206098797	-0.2217136238	-0.0528000312
C	6.0	9.7188280142	-0.1058949816	-0.1444086752
C	6.0	-8.4099175012	-0.2796095812	-0.2016256295
C	6.0	11.1072007505	-0.1496178295	-0.3064948436
H	1.0	-8.8866042725	-0.2940610001	-1.1759246161
H	1.0	11.5747407974	-0.1658378715	-1.2852468934
C	6.0	-9.1811034998	-0.3188002788	0.9637265408
C	6.0	11.8901586987	-0.1721271049	0.8514541807
H	1.0	-10.2632695659	-0.3641872357	0.8786744027
H	1.0	12.9718521678	-0.2063242176	0.7559347707
C	6.0	-8.5856752258	-0.3013914137	2.2318165102
C	6.0	11.3071209905	-0.1522599252	2.1252771567
H	1.0	-9.2083135324	-0.3332453756	3.1212394156
H	1.0	11.9385653683	-0.1708044611	3.0088446593
C	6.0	-7.1892330279	-0.2435949137	2.3597719272
C	6.0	9.9114706356	-0.1091234577	2.2665578576
H	1.0	-6.7307730333	-0.2307682387	3.3453754968
H	1.0	9.4622846314	-0.0945076900	3.2564117112
C	6.0	-6.4102122879	-0.2034324075	1.2126532451
C	6.0	9.1208513227	-0.0859778001	1.1269962097
C	6.0	-4.9006410458	-0.1404369111	1.0447410944
C	6.0	7.6089784437	-0.0418278651	0.9738863493
C	6.0	-4.2384553165	-1.3967978905	1.6679912387
C	6.0	6.9689208693	-1.3026012778	1.6111817568
C	6.0	-4.3403595651	1.1541468868	1.6886441321
C	6.0	7.0400235135	1.2498993177	1.6157374330
H	1.0	-4.6440031681	-2.3127727652	1.2265358940
H	1.0	7.3809730405	-2.2158543102	1.1700612231
H	1.0	-4.8050212135	2.0430316477	1.2500606845
H	1.0	7.4938697058	2.1412025031	1.1707736659
H	1.0	-4.4360685937	-1.4187715643	2.7453439074
H	1.0	7.1786211013	-1.3163129619	2.6863652106
H	1.0	-4.5535088380	1.1504959492	2.7631786354
H	1.0	7.2594411477	1.2527414822	2.6890193771
H	1.0	-3.1545451893	-1.3953902417	1.5225486568
H	1.0	5.8835254370	-1.3155008828	1.4778498981
H	1.0	-3.2573987472	1.2320811138	1.5591481364
H	1.0	5.9556501079	1.3173817304	1.4922152057
H	1.0	0.1572745628	0.0822522605	0.0702004704
C	6.0	1.3388309232	0.0718531613	-1.7173486311
C	6.0	2.5657872276	0.0907865753	-1.0334445237
H	1.0	2.5405674039	0.1014380372	0.0559702426
C	6.0	1.3298623797	0.0337862627	-3.2352624742
C	6.0	-1.2123242183	0.0457647122	-3.1481427445
C	6.0	3.8727430459	0.0741430426	-3.1780767455
C	6.0	2.6042136355	0.6837997379	-3.7950669615
C	6.0	0.0419356173	0.6707586069	-3.7787491831
H	1.0	3.9892786421	-0.9619109762	-3.5328950971
H	1.0	4.7529732655	0.6192996131	-3.5367580903
H	1.0	-1.3226416384	-0.9901589694	-3.5053272879
H	1.0	-2.1026512563	0.5829552980	-3.4937422586

H	1.0	1.3332268161	-1.0280392204	-3.5390959675
H	1.0	2.6314704702	0.5702535225	-4.8854946223
H	1.0	2.5793488682	1.7620974981	-3.5844469226
H	1.0	0.0030949310	0.5590213303	-4.8689879878
H	1.0	0.0575189528	1.7488537409	-3.5661863648

C



E(B3LYP-PCM): S0 = –1964.401473*
E(HOMO) = –0.1755; E(LUMO) = –0.1117

E(TDDFT-B3LYP-PCM): S1 = –1964.347435
Oscillator strength S1 → S0 = 2.9912*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
141	144	0.034802	0.022818
143	144	0.999568	-0.108149
142	145	-0.093388	-0.030896
141	148	-0.031972	-0.014406

E(ORMAS-PT2-PCM): S0 = –1959.877410*
E(ORMAS-PT2-PCM): S1 = –1959.830738

Optimized TDDFT-B3LYP-PCM geometry:

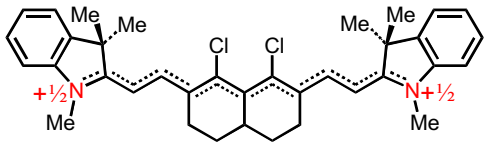
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1305381445	0.3423176177	-0.8343174718
C	6.0	-1.1491862241	0.2401055744	-1.4323901543
C	6.0	3.8510970839	0.2350171538	-1.5659315475
C	6.0	-2.3346996246	0.1666457067	-0.6804257839
C	6.0	5.0313725543	0.1836150022	-0.8017931874
H	1.0	-2.2334445798	0.2266641551	0.3947191648
H	1.0	4.8988677266	0.2492887390	0.2740008218
C	6.0	-3.6239867803	-0.0067807457	-1.2137851451
C	6.0	6.3299414125	0.0322456245	-1.3153887731
H	1.0	-3.7177514172	-0.0810485291	-2.2918707193
H	1.0	6.4279224897	-0.0444243687	-2.3936614369
C	6.0	-4.8060945296	-0.1137974156	-0.4823057652
C	6.0	7.5104917627	-0.0462054367	-0.5777968696
N	7.0	-6.0205631109	-0.2835437716	-1.0974082925
N	7.0	8.7314097675	-0.1956456851	-1.1846078838
C	6.0	-6.2045865328	-0.3460633130	-2.5419800127
C	6.0	8.9238856433	-0.2682970021	-2.6275934917
H	1.0	-7.2678235501	-0.3937678225	-2.7702161821
H	1.0	9.9887946851	-0.3041844259	-2.8502702408
H	1.0	-5.7126301345	-1.2341504507	-2.9536059789
H	1.0	8.4457813135	-1.1664286059	-3.0335687286
H	1.0	-5.7847479450	0.5483776750	-3.0125474487

H	1.0	8.4946907158	0.6162956557	-3.1083787158
C	6.0	-7.0599092889	-0.3912696054	-0.1666646893
C	6.0	9.7677253190	-0.2703583361	-0.2468207260
C	6.0	-8.4271339847	-0.5857182767	-0.3878222131
C	6.0	11.1400252122	-0.4361166519	-0.4586207793
H	1.0	-8.8437490026	-0.6816426264	-1.3847398201
H	1.0	11.5643993184	-0.5325110286	-1.4522136059
C	6.0	-9.2558403365	-0.6583780294	0.7352701750
C	6.0	11.9638944887	-0.4784593604	0.6696884419
H	1.0	-10.3223447720	-0.8103284052	0.5949312288
H	1.0	13.0343118912	-0.6076975264	0.5365244927
C	6.0	-8.7370241031	-0.5406137271	2.0315487605
C	6.0	11.4353742593	-0.3588858074	1.9617670310
H	1.0	-9.4030291371	-0.6002007567	2.8874334712
H	1.0	12.0980098892	-0.3947269188	2.8215855923
C	6.0	-7.3614618607	-0.3479444964	2.2320405533
C	6.0	10.0546848274	-0.1953370108	2.1528886911
H	1.0	-6.9639091047	-0.2589307934	3.2398559033
H	1.0	9.6495381164	-0.1049314956	3.1575596503
C	6.0	-6.5255097476	-0.2756023599	1.1273298564
C	6.0	9.2234196662	-0.1534640326	1.0430178885
C	6.0	-5.0205132753	-0.0843772824	1.0372518515
C	6.0	7.7148587609	0.0016787611	0.9422830027
C	6.0	-4.2901338760	-1.2514367019	1.7512317604
C	6.0	7.0062326507	-1.1762301461	1.6603953567
C	6.0	-4.6138516709	1.2802904139	1.6515190605
C	6.0	7.2700127521	1.3608278442	1.5419006622
H	1.0	-4.5625304092	-2.2145871233	1.3079775360
H	1.0	7.3164434354	-2.1373380571	1.2379624179
H	1.0	-5.1385080067	2.1046356702	1.1579961490
H	1.0	7.7774063801	2.1941677866	1.0454414036
H	1.0	-4.5763312136	-1.2681694533	2.8084848617
H	1.0	7.2708218147	-1.1683447408	2.7233397718
H	1.0	-4.8764021109	1.2943719853	2.7148875363
H	1.0	7.5236606386	1.3901830204	2.6071003670
H	1.0	-3.2036118842	-1.1421071500	1.6969880737
H	1.0	5.9183191007	-1.1004540316	1.5818545497
H	1.0	-3.5380975427	1.4565586635	1.5651275455
H	1.0	6.1908166515	1.5081698997	1.4455617175
C	6.0	1.3622178010	0.2987078030	-1.5280804359
C	6.0	2.6147566153	0.3295826749	-0.8947369562
H	1.0	2.6448797402	0.3970211248	0.1881693423
C	6.0	1.3205425149	0.1636122651	-3.0468899642
C	6.0	-1.1967552780	0.1682240861	-2.9504256028
C	6.0	3.8604476276	0.1612757337	-3.0777369233
C	6.0	2.5849630372	0.7644504516	-3.6765829456
C	6.0	0.0388130874	0.7776093270	-3.6129818428
H	1.0	3.9508988304	-0.8913032865	-3.3888599429
H	1.0	4.7384073550	0.6758686881	-3.4838605795
H	1.0	-1.2968655459	-0.8844331598	-3.2566298812
H	1.0	-2.0935868909	0.6807017180	-3.3131960672
H	1.0	1.3083557140	-0.9157919729	-3.2773702628

H	1.0	2.5664408261	0.5982411713	-4.7601149441
H	1.0	2.5836123466	1.8515810600	-3.5168320959
H	1.0	-0.0040008284	0.6171215671	-4.6965381071
H	1.0	0.0507570820	1.8636168776	-3.4466389068
CL	17.0	0.2050183290	0.4910536263	0.9400472126

D



E(B3LYP-PCM): S0 = –2423.908801*
E(HOMO) = –0.1781; E(LUMO) = –0.1172

E(TDDFT-B3LYP-PCM): S1 = –2423.857893
Oscillator strength S1 → S0 = 2.7141*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
151	152	1.000051	-0.107554
150	153	-0.085876	-0.030891

E(ORMAS-PT2-PCM): S0 = –2418.892502*
E(ORMAS-PT2-PCM): S1 = –2418.849542

Optimized TDDFT-B3LYP-PCM geometry:

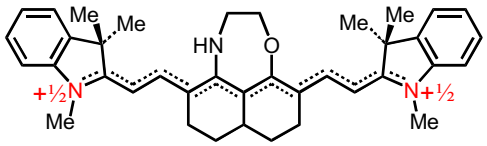
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0840352461	0.0337675554	-0.5196633279
C	6.0	-1.1532753144	0.2412146361	-1.1529580245
C	6.0	3.8531764437	0.0305074652	-1.2573559017
C	6.0	-2.3913168933	0.0092643937	-0.5032039825
C	6.0	5.0939549891	0.1408014641	-0.6284214641
H	1.0	-2.3495279282	-0.3084803794	0.5291789587
H	1.0	5.0970695451	0.5214030950	0.3840041460
C	6.0	-3.6437822884	0.1556211566	-1.1054685963
C	6.0	6.3336919686	-0.2346846315	-1.1909802536
H	1.0	-3.6734004581	0.4569978542	-2.1471194458
H	1.0	6.3278229725	-0.6494821693	-2.1928204898
C	6.0	-4.8842728869	-0.0618454505	-0.4944289901
C	6.0	7.5744432365	-0.1415487202	-0.5712835801
N	7.0	-6.0549254957	0.0941890669	-1.1819848557
N	7.0	8.7231028013	-0.5561694972	-1.1993733459
C	6.0	-6.1374908256	0.4818406144	-2.5862170707
C	6.0	8.7592728215	-1.1289876656	-2.5396285602
H	1.0	-7.1806794684	0.5023955324	-2.8954103830
H	1.0	9.7854330727	-1.3828400705	-2.7983517159
H	1.0	-5.5993370723	-0.2398951945	-3.2085167240
H	1.0	8.1494870354	-2.0373937836	-2.5776759186
H	1.0	-5.7059257946	1.4775671170	-2.7307217250
H	1.0	8.3783297415	-0.4077526517	-3.2700622989
C	6.0	-7.1695691655	-0.1590658884	-0.3696492756

C	6.0	9.8499970218	-0.3655590315	-0.3934068838
C	6.0	-8.5275901762	-0.1061625179	-0.6948484366
C	6.0	11.1904370848	-0.6549524444	-0.6684287154
H	1.0	-8.8760600904	0.1582626097	-1.6873917722
H	1.0	11.5065641540	-1.0918382405	-1.6094852093
C	6.0	-9.4418136813	-0.4104984500	0.3177744219
C	6.0	12.1281143000	-0.3581459514	0.3239835987
H	1.0	-10.5048114521	-0.3785797679	0.0959691784
H	1.0	13.1772585397	-0.5712717415	0.1394358936
C	6.0	-9.0120502644	-0.7537979827	1.6063642201
C	6.0	11.7398921852	0.2065302862	1.5464575034
H	1.0	-9.7438581656	-0.9855120753	2.3747630104
H	1.0	12.4897039615	0.4271139089	2.3005742790
C	6.0	-7.6433774155	-0.8005208451	1.9117118500
C	6.0	10.3892621220	0.4887949962	1.8031828240
H	1.0	-7.3155484111	-1.0673524657	2.9131135681
H	1.0	10.0935779362	0.9269546863	2.7529249416
C	6.0	-6.7237963425	-0.5009210265	0.9166159627
C	6.0	9.4462907676	0.2001679340	0.8275692871
C	6.0	-5.2048570645	-0.4725274299	0.9480202078
C	6.0	7.9389455780	0.3935794019	0.8212128978
C	6.0	-4.6502633571	-1.8810456980	1.2882769856
C	6.0	7.2880031858	-0.4411702140	1.9545181321
C	6.0	-4.7054076753	0.5802281602	1.9716919768
C	6.0	7.5898109774	1.8969740632	0.9704905000
H	1.0	-5.0035180972	-2.6260938606	0.5684049448
H	1.0	7.5229407707	-1.5044448537	1.8435388876
H	1.0	-5.0879491820	1.5764697026	1.7281715217
H	1.0	8.0541726565	2.4879065675	0.1746035265
H	1.0	-4.9962979090	-2.1751901869	2.2847430490
H	1.0	7.6732347061	-0.1036339126	2.9227064899
H	1.0	-5.0591157293	0.3116739725	2.9727418543
H	1.0	7.9631858799	2.2643663485	1.9323210752
H	1.0	-3.5568468349	-1.8954137186	1.2910833150
H	1.0	6.2003735359	-0.3281430530	1.9670426686
H	1.0	-3.6132632175	0.6282759452	2.0001286484
H	1.0	6.5096212285	2.0659097491	0.9388755361
C	6.0	1.3561601849	0.1527378734	-1.1742045597
C	6.0	2.6175998243	0.3272245227	-0.5919274129
C	6.0	1.2684778281	0.0826374645	-2.7025942785
C	6.0	-1.1727268796	0.7146874768	-2.5980248745
C	6.0	3.7237315227	-0.4465319856	-2.6893209444
C	6.0	2.6088308224	0.3275050236	-3.3918694190
C	6.0	0.1990701890	1.0885812503	-3.1535739702
H	1.0	3.4995052441	-1.5238573279	-2.7113030429
H	1.0	4.6654121221	-0.3091929491	-3.2255388877
H	1.0	-1.6025382456	-0.0933717767	-3.2086433216
H	1.0	-1.8583229168	1.5650544436	-2.6936041240
H	1.0	0.9239643692	-0.9293619102	-2.9692322593
H	1.0	2.5331444133	0.0258950841	-4.4426938981
H	1.0	2.8479729084	1.3994915569	-3.3779219721
H	1.0	0.1583681540	1.1170866064	-4.2491207968

H	1.0	0.4909488162	2.0911173114	-2.8151647021
CL	17.0	0.0485286488	-0.6099250838	1.1372530506
CL	17.0	2.7382503060	0.9878624864	1.0526062996

E



E(B3LYP-PCM): S0 = –1712.741846*
E(HOMO) = –0.1723; E(LUMO) = –0.0931

E(TDDFT-B3LYP-PCM): S1 = –1712.677813
Oscillator strength S1 → S0 = 2.4892*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
149	151	-0.035290	-0.003764
150	151	0.995293	-0.062201
149	152	-0.084691	-0.007228
148	155	0.032730	0.011502

E(ORMAS-PT2-PCM): S0 = –1708.225372*
E(ORMAS-PT2-PCM): S1 = –1708.166961

Optimized TDDFT-B3LYP-PCM geometry:

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1336246452	-0.8930887391	-0.8285153789
C	6.0	-1.0596748295	-0.4054635030	-1.4660643847
C	6.0	3.8988389346	-0.9295857933	-1.5237662110
C	6.0	-2.2589061766	-0.3487119875	-0.7500711003
C	6.0	5.0508063254	-0.6362648252	-0.7909949819
H	1.0	-2.2282367851	-0.7279930684	0.2621473325
H	1.0	4.9536007110	-0.5689278688	0.2871035790
C	6.0	-3.4788106584	0.1759075978	-1.2355771136
C	6.0	6.3158560540	-0.3484724409	-1.3624342502
H	1.0	-3.4808943244	0.5889487396	-2.2393291041
H	1.0	6.4000075411	-0.4513949554	-2.4393106158
C	6.0	-4.6845389623	0.2239494794	-0.5478382406
C	6.0	7.4605865533	0.0592892364	-0.6958289567
N	7.0	-5.8204432878	0.7662101387	-1.1097714689
N	7.0	8.6395056685	0.3094847478	-1.3673585337
C	6.0	-5.8680405631	1.3537093957	-2.4408979318
C	6.0	8.8038880799	0.1538600624	-2.8049253126
H	1.0	-6.8687767234	1.7358179539	-2.6350342940
H	1.0	9.8374602098	0.3611180057	-3.0773983649
H	1.0	-5.6238727509	0.6026894014	-3.2004185941
H	1.0	8.5614294981	-0.8711857208	-3.1051204764
H	1.0	-5.1542504855	2.1810899371	-2.5144733709

H	1.0	8.1497608258	0.8478745791	-3.3447602068
C	6.0	-6.9143490522	0.6803805146	-0.2445274844
C	6.0	9.6474811965	0.7351544723	-0.4972504679
C	6.0	-8.2328180592	1.1051832152	-0.4405690770
C	6.0	10.9654779086	1.1036447747	-0.7843720553
H	1.0	-8.5557442227	1.5801035259	-1.3609238858
H	1.0	11.3612464003	1.0927698944	-1.7944878343
C	6.0	-9.1398624979	0.8949462033	0.6020926696
C	6.0	11.7738337825	1.4983690299	0.2865117977
H	1.0	-10.1706121651	1.2149172499	0.4764130188
H	1.0	12.8019528022	1.7907662873	0.0910313835
C	6.0	-8.7451186582	0.2820403774	1.7983435415
C	6.0	11.2835046096	1.5231864873	1.5980406121
H	1.0	-9.4702533510	0.1302289647	2.5926173726
H	1.0	11.9321030425	1.8337686958	2.4121348320
C	6.0	-7.4170908720	-0.1373529446	1.9758564215
C	6.0	9.9565309555	1.1511272720	1.8653445057
H	1.0	-7.1139699936	-0.6122820977	2.9056841456
H	1.0	9.5779816689	1.1732304525	2.8843632444
C	6.0	-6.5048674418	0.0643806884	0.9506537842
C	6.0	9.1415399929	0.7595528768	0.8132541067
C	6.0	-5.0252639813	-0.2735636182	0.8645596561
C	6.0	7.6850617403	0.3208835437	0.8017766269
C	6.0	-4.8092284481	-1.8016856453	1.0123892634
C	6.0	7.5044745003	-0.9669305984	1.6447949708
C	6.0	-4.2368947316	0.5001475636	1.9534778266
C	6.0	6.7763310363	1.4575813009	1.3343890941
H	1.0	-5.3546480700	-2.3513781409	0.2385020958
H	1.0	8.1372313586	-1.7760017659	1.2660120926
H	1.0	-4.4019419809	1.5787370274	1.8635783767
H	1.0	6.9050102129	2.3712423936	0.7449379588
H	1.0	-5.1765164240	-2.1318789826	1.9903228634
H	1.0	7.7859385505	-0.7694199684	2.6850247723
H	1.0	-4.5748703180	0.1830078646	2.9462500254
H	1.0	7.0385977976	1.6819432638	2.3742900978
H	1.0	-3.7505895199	-2.0648097059	0.9408568469
H	1.0	6.4658978668	-1.3089151756	1.6359079317
H	1.0	-3.1625074394	0.3096976045	1.8830529142
H	1.0	5.7200083606	1.1756231362	1.3048023176
C	6.0	1.4022577284	-0.9445767505	-1.4507122290
C	6.0	2.6648092915	-1.2717298044	-0.8411590950
C	6.0	1.4708969397	-0.5053932183	-2.9216298841
C	6.0	-0.9775705016	0.0498864682	-2.9035982070
C	6.0	3.9355018459	-0.8709923924	-3.0357989851
O	8.0	-0.0735400236	-1.2000633486	0.4950829419
N	7.0	2.8484359099	-1.8776691215	0.3825450941
C	6.0	0.1336080010	-0.6905229211	-3.6389052847
C	6.0	2.5940625381	-1.2454280460	-3.6505530282
H	1.0	-0.7838915890	1.1336890776	-2.9455809680
H	1.0	-1.9347173585	-0.1126619649	-3.4091052006
H	1.0	0.2220812894	-0.3208378513	-4.6674199595
H	1.0	-0.1090794698	-1.7608716304	-3.6979245211

H	1.0	1.7092148649	0.5726081183	-2.9501600943
H	1.0	2.5835365878	-0.9859783795	-4.7158723037
H	1.0	2.4230474853	-2.3280063240	-3.5760627459
H	1.0	4.2142883877	0.1436812705	-3.3573296888
H	1.0	4.7271626267	-1.5342522166	-3.4115273547
C	6.0	0.5353487264	-2.3627937535	1.0526810747
C	6.0	1.9449003059	-2.0420780236	1.5021403845
H	1.0	3.7749917970	-2.2521433265	0.5232840399
H	1.0	2.3327152809	-2.8605400928	2.1170273803
H	1.0	1.9070241049	-1.1401700225	2.1323442209
H	1.0	-0.0791523900	-2.6328365321	1.9163902762
H	1.0	0.5222857353	-3.1888062336	0.3309515656

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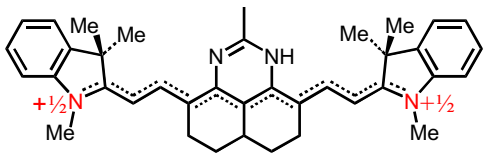


E(B3LYP-PCM): S0 = –1691.722383*
E(HOMO) = –0.1739; E(LUMO) = –0.0928

E(TDDFT-B3LYP-PCM): S1 = –1691.656597
Oscillator strength S1 → S0 = 2.5979*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
148	150	0.040542	-0.001571
149	150	0.995051	-0.058699
148	151	-0.074143	-0.001806
148	152	-0.036023	-0.005809
147	155	0.032505	0.011832

E(ORMAS-PT2-PCM): S0 = –1687.260251*
E(ORMAS-PT2-PCM): S1 = –1687.200039

Optimized TDDFT-B3LYP-PCM geometry:

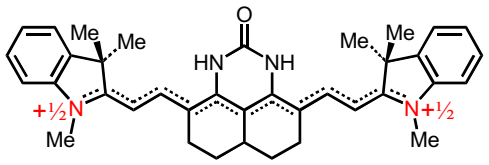
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1414890520	0.5199833167	-0.8466412045
C	6.0	-1.1459023891	0.3817358132	-1.4400817121
C	6.0	3.8426846808	0.2406967209	-1.5376050661
C	6.0	-2.3064248366	0.2371965229	-0.6681813499
C	6.0	5.0216776416	0.1920339128	-0.7957349196
H	1.0	-2.2003943376	0.1851845662	0.4103767530
H	1.0	4.9038872797	0.3249073309	0.2722468850
C	6.0	-3.6102809038	0.0806870424	-1.1931939142
C	6.0	6.3159822209	-0.0318388876	-1.3220974863
H	1.0	-3.7088482880	0.1169315812	-2.2729012131
H	1.0	6.4013457021	-0.1596729379	-2.3967123194
C	6.0	-4.7837080227	-0.1282851158	-0.4808594150
C	6.0	7.4953022014	-0.1202071253	-0.5954445049
N	7.0	-5.9996796143	-0.2726105972	-1.1168176127
N	7.0	8.7135401058	-0.3273001524	-1.2067946244
C	6.0	-6.1749574587	-0.2093501793	-2.5601459662
C	6.0	8.8937490183	-0.4441609658	-2.6467119054
H	1.0	-7.2321369935	-0.3049611791	-2.8023190303
H	1.0	9.9570049829	-0.4856442011	-2.8775516889
H	1.0	-5.6252943471	-1.0208186175	-3.0502825328
H	1.0	8.4124404330	-1.3533687986	-3.0248667050

H	1.0	-5.8126133555	0.7502484535	-2.9442106843
H	1.0	8.4604424045	0.4254822055	-3.1508487115
C	6.0	-7.0357512292	-0.4870936345	-0.2037178104
C	6.0	9.7491761148	-0.4152977106	-0.2734659478
C	6.0	-8.3994126438	-0.6883534202	-0.4422627023
C	6.0	11.1145126635	-0.6351895267	-0.4861714908
H	1.0	-8.8154003709	-0.7010145749	-1.4442150447
H	1.0	11.5287576580	-0.7734145474	-1.4791991205
C	6.0	-9.2279461665	-0.8780498716	0.6681405958
C	6.0	11.9437658737	-0.6771073290	0.6383226768
H	1.0	-10.2913293300	-1.0366622447	0.5107348757
H	1.0	13.0081567244	-0.8476955618	0.5024278619
C	6.0	-8.7142970244	-0.8667337379	1.9711027584
C	6.0	11.4284800353	-0.5060842508	1.9297569233
H	1.0	-9.3797817921	-1.0151637112	2.8165884301
H	1.0	12.0944163322	-0.5433713707	2.7869927907
C	6.0	-7.3422153949	-0.6658581327	2.1896004940
C	6.0	10.0549756130	-0.2889176844	2.1225350051
H	1.0	-6.9453617719	-0.6590108052	3.2018238926
H	1.0	9.6594468574	-0.1584542482	3.1267615395
C	6.0	-6.5071171310	-0.4786910098	1.0982221049
C	6.0	9.2183059470	-0.2456188666	1.0170129153
C	6.0	-5.0058987921	-0.2466838898	1.0339136900
C	6.0	7.7151945547	-0.0361108221	0.9220991942
C	6.0	-4.2511979828	-1.4581853610	1.6388080846
C	6.0	6.9675174283	-1.1642654685	1.6782221684
C	6.0	-4.6341912214	1.0626758694	1.7753782431
C	6.0	7.3299750571	1.3548810043	1.4883198653
H	1.0	-4.5123395689	-2.3829029798	1.1142296235
H	1.0	7.2444259451	-2.1481407180	1.2856550240
H	1.0	-5.1804741172	1.9157888406	1.3605309509
H	1.0	7.8672644044	2.1533202054	0.9662526433
H	1.0	-4.5256390417	-1.5727190681	2.6932153244
H	1.0	7.2324997010	-1.1331738202	2.7408254330
H	1.0	-4.8924145782	0.9720789072	2.8362335240
H	1.0	7.5931872839	1.4024541408	2.5507331905
H	1.0	-3.1668676273	-1.3277012918	1.5842257299
H	1.0	5.8830915771	-1.0530924444	1.5948113877
H	1.0	-3.5640228995	1.2762254821	1.7048672068
H	1.0	6.2571655471	1.5439443304	1.3949467315
C	6.0	1.3540947825	0.3920240118	-1.5607714851
C	6.0	2.5812459858	0.4296149344	-0.8652735017
C	6.0	1.3088782049	0.1890495303	-3.0592409780
C	6.0	-1.2140505527	0.3327574805	-2.9569823632
C	6.0	3.8311522049	0.0588453945	-3.0419485158
C	6.0	2.6044143402	0.6979210469	-3.7001399108
C	6.0	0.0545328368	0.8548151951	-3.6362023136
H	1.0	3.8491640460	-1.0170672197	-3.2791950966
H	1.0	4.7414720672	0.4802571767	-3.4818702591
H	1.0	-1.4042053487	-0.7031369349	-3.2780946805
H	1.0	-2.0730612452	0.9181298198	-3.3054694190
H	1.0	1.2384154349	-0.8955365092	-3.2528976207

H	1.0	2.5976722092	0.4789131051	-4.7742994578
H	1.0	2.6546162269	1.7903873898	-3.5925138675
H	1.0	-0.0006047126	0.6723483785	-4.7157135174
H	1.0	0.1296113182	1.9419086247	-3.4953907290
N	7.0	0.2760690732	0.7381949255	0.5318788369
N	7.0	2.6169511643	0.6273443747	0.5196075600
C	6.0	1.4970873997	0.7892592824	1.1522153427
C	6.0	1.4780237404	1.0428541510	2.6337229062
H	1.0	0.9160075171	0.2599435307	3.1568653734
H	1.0	0.9972938841	2.0030902481	2.8572387860
H	1.0	2.5011793078	1.0611255904	3.0111689171
H	1.0	-0.5411085750	0.9860824563	1.0719064890

G



E(B3LYP-PCM): S0 = –1727.649223*
E(HOMO) = –0.1778; E(LUMO) = –0.1012

E(TDDFT-B3LYP-PCM): S1 = –1727.586955
Oscillator strength S1 → S0 = 2.6916*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
149	150	0.996218	-0.067464
148	151	0.088026	0.009986
147	154	-0.034175	-0.013152

E(ORMAS-PT2-PCM): S0 = –1723.145973*
E(ORMAS-PT2-PCM): S1 = –1723.092012

Optimized TDDFT-B3LYP-PCM geometry:

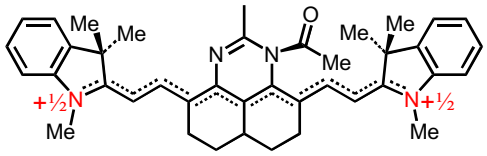
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1064592767	0.8475380775	-0.9033431611
C	6.0	-1.1599902605	0.5449055969	-1.4887138514
C	6.0	3.8156366275	0.5786957655	-1.5172207330
C	6.0	-2.3140285839	0.3916055792	-0.7110990828
C	6.0	4.9806188519	0.4419168510	-0.7530678230
H	1.0	-2.2177730653	0.4634194580	0.3667915864
H	1.0	4.8961432872	0.5132239199	0.3259036098
C	6.0	-3.5926517990	0.0777158701	-1.2251810157
C	6.0	6.2571858061	0.1443634915	-1.2816729985
H	1.0	-3.6823056761	0.0053701359	-2.3035962175
H	1.0	6.3348124695	0.0710133355	-2.3609814872
C	6.0	-4.7517686546	-0.1643702973	-0.4982114491
C	6.0	7.4278269035	-0.0813755320	-0.5681225508
N	7.0	-5.9403421013	-0.4724053000	-1.1212024839
N	7.0	8.6130709667	-0.3744087694	-1.2045792743
C	6.0	-6.1015633717	-0.5772222500	-2.5649718535
C	6.0	8.7598736561	-0.4700662303	-2.6505312539
H	1.0	-7.1254643126	-0.8655040427	-2.7959154517
H	1.0	9.7898143231	-0.7227524580	-2.8958386853
H	1.0	-5.4232254513	-1.3369362213	-2.9673842991
H	1.0	8.1013915461	-1.2497326991	-3.0480063079
H	1.0	-5.8881468022	0.3843998475	-3.0443953026

H	1.0	8.5093378855	0.4859614071	-3.1229429196
C	6.0	-6.9678717971	-0.6800376542	-0.1967070854
C	6.0	9.6524621175	-0.5742102000	-0.2916567674
C	6.0	-8.3100474789	-1.0029218910	-0.4237742197
C	6.0	10.9942791367	-0.8876639442	-0.5334705135
H	1.0	-8.7121495393	-1.1309959974	-1.4230567089
H	1.0	11.3859050431	-1.0151034960	-1.5370014789
C	6.0	-9.1338360047	-1.1562476686	0.6949014481
C	6.0	11.8317647245	-1.0335998215	0.5760146086
H	1.0	-10.1806357523	-1.4075985913	0.5484842119
H	1.0	12.8786302029	-1.2776753973	0.4181047055
C	6.0	-8.6356756964	-0.9928437230	1.9940995026
C	6.0	11.3472561344	-0.8718435563	1.8806142424
H	1.0	-9.2971269398	-1.1175927817	2.8464704418
H	1.0	12.0194541699	-0.9901934286	2.7254696718
C	6.0	-7.2861015962	-0.6668506074	2.2009403851
C	6.0	9.9974806696	-0.5568921104	2.1023281501
H	1.0	-6.9041128502	-0.5396516451	3.2107031818
H	1.0	9.6257850400	-0.4318997912	3.1162109562
C	6.0	-6.4558296688	-0.5113077246	1.1008363321
C	6.0	9.1535245628	-0.4097722274	1.0115386322
C	6.0	-4.9793327434	-0.1594807645	1.0202467553
C	6.0	7.6727710556	-0.0728295098	0.9476398359
C	6.0	-4.1282596835	-1.2383364143	1.7376601753
C	6.0	6.8417351984	-1.1594142654	1.6766594841
C	6.0	-4.7299279735	1.2408914320	1.6364212559
C	6.0	7.4161124120	1.3259658485	1.5645262658
H	1.0	-4.2942740557	-2.2264932805	1.2970271354
H	1.0	7.0132046810	-2.1464122797	1.2355083174
H	1.0	-5.3340616387	2.0036864367	1.1350815500
H	1.0	8.0085059016	2.0936061973	1.0565876698
H	1.0	-4.4094766851	-1.2828658847	2.7955387469
H	1.0	7.1360108208	-1.1992403759	2.7311797118
H	1.0	-5.0023408811	1.2300101513	2.6974604547
H	1.0	7.6985584523	1.3189496166	2.6229718182
H	1.0	-3.0597686231	-1.0126160210	1.6810838052
H	1.0	5.7702144018	-0.9455927804	1.6327175709
H	1.0	-3.6786990520	1.5321868521	1.5616552612
H	1.0	6.3615885015	1.6075036891	1.4991047303
C	6.0	1.3263633527	0.7028997971	-1.5950462423
C	6.0	2.5520741586	0.8643293539	-0.9174437426
C	6.0	1.3205525394	0.3196849196	-3.0579742150
C	6.0	-1.2052953814	0.3192329059	-2.9899458133
C	6.0	3.8468016181	0.3532318044	-3.0189204553
C	6.0	2.5886294786	0.8512987223	-3.7333288406
C	6.0	0.0378146134	0.8341920501	-3.7186640058
H	1.0	3.9804185439	-0.7210205651	-3.2191707900
H	1.0	4.7243464693	0.8514672307	-3.4471976250
H	1.0	-1.3265393427	-0.7567557746	-3.1886958101
H	1.0	-2.0943372915	0.8054951982	-3.4081302912
H	1.0	1.3274196947	-0.7814826893	-3.1339578873
H	1.0	2.6110555025	0.5359284819	-4.7829373658

H	1.0	2.5656023736	1.9495944388	-3.7245050062
H	1.0	0.0076968619	0.5184405948	-4.7679501193
H	1.0	0.0462272523	1.9326889815	-3.7100394141
N	7.0	2.4923011769	1.2533682400	0.4297806927
N	7.0	0.1763955367	1.2371646565	0.4432808503
C	6.0	1.3364066014	1.5275040323	1.1266220515
O	8.0	1.3398825269	1.9840068277	2.2671367048
H	1.0	3.3309314587	1.5710133544	0.8958340648
H	1.0	-0.6610745910	1.5434758329	0.9188537447

H



E(B3LYP-PCM): S0 = –1844.262776*
E(HOMO) = –0.1749; E(LUMO) = –0.1086

E(TDDFT-B3LYP-PCM): S1 = –1844.208165
Oscillator strength S1 → S0 = 2.4791*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
160	161	0.998489	-0.090869
159	162	0.077495	0.018027
159	163	0.031085	0.008778

E(ORMAS-PT2-PCM): S0 = –1839.443790*
E(ORMAS-PT2-PCM): S1 = –1839.397449

Optimized TDDFT-B3LYP-PCM geometry:

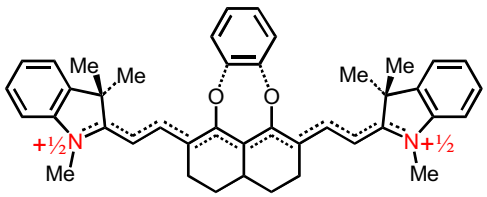
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1228171765	0.8575435193	-1.0414177632
C	6.0	-1.1548301239	0.5389397329	-1.6018360689
C	6.0	3.7892507863	0.3171621645	-1.5913564732
C	6.0	-2.2814093020	0.3578022089	-0.7968307349
C	6.0	4.9378363432	0.1726532192	-0.8083314616
H	1.0	-2.1393752118	0.4537959547	0.2738842095
H	1.0	4.7809176491	0.2267879003	0.2621980674
C	6.0	-3.5658414412	0.0123644540	-1.2678374783
C	6.0	6.2365376721	-0.0575768157	-1.3062713057
H	1.0	-3.6959211494	-0.0586518659	-2.3426288210
H	1.0	6.3512559784	-0.1272893499	-2.3832948603
C	6.0	-4.6884246301	-0.2487963931	-0.4898315453
C	6.0	7.3938880450	-0.2154872100	-0.5512454005
N	7.0	-5.8973995792	-0.5679307043	-1.0580115806
N	7.0	8.6127001549	-0.4549422614	-1.1377827330
C	6.0	-6.1245483511	-0.6668402444	-2.4941212311
C	6.0	8.8166354581	-0.5828999047	-2.5748472628
H	1.0	-7.1490674084	-0.9855653379	-2.6769994084
H	1.0	9.8520806307	-0.8555142852	-2.7710157669
H	1.0	-5.4440354365	-1.4032528191	-2.9335057171
H	1.0	8.1657931936	-1.3647689990	-2.9788980020
H	1.0	-5.9632943405	0.3043000613	-2.9743481475
H	1.0	8.5964312503	0.3641380382	-3.0797955834

C	6.0	-6.8815365900	-0.7867150009	-0.0879879448
C	6.0	9.6324188375	-0.5575324808	-0.1845401135
C	6.0	-8.2294020808	-1.1182136249	-0.2577749939
C	6.0	10.9986662734	-0.7854949950	-0.3748312789
H	1.0	-8.6743311494	-1.2451398982	-1.2388119326
H	1.0	11.4317126030	-0.9095400157	-1.3616042964
C	6.0	-9.0015662647	-1.2821772751	0.8956793603
C	6.0	11.8062183685	-0.8462474128	0.7648275837
H	1.0	-10.0520688403	-1.5399256452	0.7943989402
H	1.0	12.8717776914	-1.0225802804	0.6471410225
C	6.0	-8.4467485806	-1.1201438767	2.1717327998
C	6.0	11.2676188280	-0.6835735335	2.0475045085
H	1.0	-9.0684978073	-1.2531022593	3.0522769312
H	1.0	11.9168046736	-0.7349161541	2.9167721360
C	6.0	-7.0918632345	-0.7847531337	2.3205071244
C	6.0	9.8932817393	-0.4538508903	2.2169236699
H	1.0	-6.6663583863	-0.6590209770	3.3128126879
H	1.0	9.4802715530	-0.3276451088	3.2145426608
C	6.0	-6.3125847206	-0.6176575121	1.1849542457
C	6.0	9.0787311974	-0.3905807187	1.0955467196
C	6.0	-4.8419628542	-0.2607055490	1.0385265162
C	6.0	7.5808650047	-0.1612895763	0.9716526497
C	6.0	-3.9568372294	-1.3535709881	1.6918988986
C	6.0	6.8031352294	-1.2953573572	1.6880571732
C	6.0	-4.5623816414	1.1264895045	1.6719328027
C	6.0	7.1971352223	1.2236180504	1.5519344360
H	1.0	-4.1616806651	-2.3368002560	1.2565631469
H	1.0	7.0789737812	-2.2750228624	1.2846270802
H	1.0	-5.1547634742	1.9081395656	1.1858634216
H	1.0	7.7539310056	2.0247868216	1.0552652286
H	1.0	-4.1679428950	-1.4029857171	2.7656536093
H	1.0	7.0427993744	-1.2856830912	2.7569516174
H	1.0	-4.8330692651	1.1032061412	2.7331785799
H	1.0	7.4364086991	1.2513262720	2.6205496496
H	1.0	-2.8924450801	-1.1370896597	1.5645186877
H	1.0	5.7222709735	-1.1707513715	1.5806535470
H	1.0	-3.5055198106	1.4004124837	1.6061514802
H	1.0	6.1285955759	1.4247175514	1.4371873223
C	6.0	1.3154940659	0.5722853760	-1.7133301616
C	6.0	2.5165257470	0.5029777202	-0.9650097504
C	6.0	1.3120552649	0.2618336406	-3.1913113490
C	6.0	-1.2100899120	0.3069384070	-3.1022238219
C	6.0	3.8465222463	0.2462651000	-3.1067823455
C	6.0	2.6051188299	0.8208560794	-3.8027187909
C	6.0	0.0367879217	0.8129232156	-3.8367440400
H	1.0	3.9700190068	-0.8072546823	-3.4039094945
H	1.0	4.7384448738	0.7675071404	-3.4733179407
H	1.0	-1.3366908515	-0.7694140710	-3.2939847456
H	1.0	-2.1013162934	0.7942098978	-3.5161720794
H	1.0	1.3189687937	-0.8341654277	-3.3202348817
H	1.0	2.6425757380	0.5910974983	-4.8739901432
H	1.0	2.5990299798	1.9153651710	-3.7070274337

H	1.0	-0.0098735823	0.5185297894	-4.8912070975
H	1.0	0.0638590993	1.9110655224	-3.8081876998
N	7.0	0.2380987064	1.3374773168	0.3017611079
N	7.0	2.4395571744	0.4843972538	0.4237097612
C	6.0	1.3663872031	0.8547788440	1.0362469330
C	6.0	1.2981773443	0.7508255167	2.5330185220
H	1.0	0.3637463632	0.2801742061	2.8533730765
H	1.0	1.3357645887	1.7367563109	3.0039878621
H	1.0	2.1506672966	0.1556873795	2.8682708536
C	6.0	-0.4878569849	2.4703774722	0.7536235421
C	6.0	-1.1331246425	3.3565768842	-0.2938450799
H	1.0	-0.5704012461	3.3779392271	-1.2302871023
H	1.0	-1.1871733760	4.3601243355	0.1342893392
H	1.0	-2.1522811514	3.0269620726	-0.5197782598
O	8.0	-0.5523587595	2.7480853916	1.9434621312

I



E(B3LYP-PCM): S0 = –1884.936684*
E(HOMO) = –0.1761; E(LUMO) = –0.1072

E(TDDFT-B3LYP-PCM): S1 = –1884.879539
Oscillator strength S1 → S0 = 2.9015*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
162	163	0.997680	-0.090094
161	164	0.094669	0.023601

E(ORMAS-PT2-PCM): S0 = –1880.037838*
E(ORMAS-PT2-PCM): S1 = –1879.990385

Optimized TDDFT-B3LYP-PCM geometry:

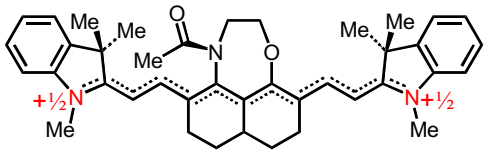
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0796840283	0.5033575588	-0.8011569215
C	6.0	-1.1665262709	0.3720854478	-1.4746195840
C	6.0	3.8377703599	0.4136965170	-1.5007268441
C	6.0	-2.3477023442	0.1664473247	-0.7442403904
C	6.0	5.0296843760	0.2226591125	-0.7835948023
H	1.0	-2.2510844196	0.1537536356	0.3329020204
H	1.0	4.9442174507	0.1958050129	0.2942355921
C	6.0	-3.6164422666	-0.0544646963	-1.3132309005
C	6.0	6.2973111049	0.0366050715	-1.3672107670
H	1.0	-3.6831744683	-0.0622521179	-2.3961374949
H	1.0	6.3543575001	0.0498235579	-2.4506102991
C	6.0	-4.8033070917	-0.2839860347	-0.6221292604
C	6.0	7.4949476668	-0.1814318245	-0.6910597587
N	7.0	-5.9893684279	-0.5014758240	-1.2800735249
N	7.0	8.6808038359	-0.3507779486	-1.3631786313
C	6.0	-6.1280811367	-0.5091161402	-2.7308435389
C	6.0	8.8121799464	-0.3050954867	-2.8138650320
H	1.0	-7.1675173868	-0.6939690945	-2.9957962879
H	1.0	9.8618499667	-0.4024336063	-3.0846747344
H	1.0	-5.5060058431	-1.2973485975	-3.1678421009
H	1.0	8.2492197574	-1.1235391488	-3.2756224784
H	1.0	-5.8253113814	0.4583314473	-3.1450007772

H	1.0	8.4376823597	0.6498198618	-3.1963409924
C	6.0	-7.0449486819	-0.7098876375	-0.3860256481
C	6.0	9.7461893120	-0.5694858801	-0.4832131733
C	6.0	-8.3936155018	-0.9655796896	-0.6542706270
C	6.0	11.0969259532	-0.7922540719	-0.7695792682
H	1.0	-8.7793654980	-1.0340781172	-1.6658039274
H	1.0	11.4756001402	-0.8244046810	-1.7855998509
C	6.0	-9.2465067951	-1.1340383676	0.4402537324
C	6.0	11.9613743021	-0.9787527203	0.3128271752
H	1.0	-10.2995058653	-1.3339801739	0.2624604438
H	1.0	13.0164314213	-1.1534476203	0.1209312630
C	6.0	-8.7695211873	-1.0492262226	1.7549352023
C	6.0	11.4931819359	-0.9439738298	1.6328576979
H	1.0	-9.4541240168	-1.1828882629	2.5874820020
H	1.0	12.1867624632	-1.0908355086	2.4557130078
C	6.0	-7.4119949219	-0.7935227853	2.0029317514
C	6.0	10.1330069731	-0.7220612058	1.8989430112
H	1.0	-7.0461522642	-0.7292089806	3.0245659095
H	1.0	9.7742865587	-0.6968338361	2.9248129729
C	6.0	-6.5526519265	-0.6260578724	0.9270576987
C	6.0	9.2621250463	-0.5370809888	0.8351512359
C	6.0	-5.0592234247	-0.3467039567	0.8902157257
C	6.0	7.7634532427	-0.2850545502	0.8169414273
C	6.0	-4.2807140004	-1.5062517134	1.5638564368
C	6.0	7.0111966686	-1.4793192332	1.4590430213
C	6.0	-4.7476211701	1.0042645564	1.5837852331
C	6.0	7.4318177464	1.0372014228	1.5554942915
H	1.0	-4.4956429824	-2.4602031533	1.0719148691
H	1.0	7.2435738617	-2.4139191970	0.9386697237
H	1.0	-5.3012478066	1.8235183663	1.1141425282
H	1.0	7.9683649222	1.8810159658	1.1102515626
H	1.0	-4.5824978578	-1.5862422206	2.6139211878
H	1.0	7.3181527986	-1.5836181449	2.5054115851
H	1.0	-5.0400326749	0.9523514247	2.6382531820
H	1.0	7.7307809460	0.9553784942	2.6061564828
H	1.0	-3.2006560447	-1.3385245815	1.5338518789
H	1.0	5.9279514625	-1.3322776111	1.4368113949
H	1.0	-3.6807239322	1.2413984884	1.5396935866
H	1.0	6.3607119922	1.2569448494	1.5246758743
C	6.0	1.3343880382	0.5522097988	-1.4525953500
C	6.0	2.5966415308	0.5208522546	-0.8143923167
C	6.0	1.3270204017	0.5288593761	-2.9812211394
C	6.0	-1.1805503830	0.4290489872	-2.9874418965
C	6.0	3.8361719935	0.4796328016	-3.0133930677
C	6.0	2.5891831739	1.1796904928	-3.5492134106
C	6.0	0.0464452487	1.1529784856	-3.5376910925
H	1.0	3.8918251633	-0.5385938150	-3.4292539879
H	1.0	4.7332232412	1.0026222677	-3.3616998631
H	1.0	-1.2178542506	-0.5923296453	-3.3977885926
H	1.0	-2.0919133840	0.9307073396	-3.3297951580
H	1.0	1.3364394981	-0.5310997767	-3.2906949699
H	1.0	2.5693126063	1.1241569354	-4.6438588413

H	1.0	2.6101167866	2.2436833824	-3.2761981285
H	1.0	0.0565238176	1.0952129292	-4.6323461026
H	1.0	0.0067419872	2.2169234946	-3.2667438589
O	8.0	-0.0277919080	0.4651221738	0.5855137416
O	8.0	2.7173226178	0.4778740948	0.5711495524
C	6.0	0.6475049639	1.3996675048	1.3457315953
C	6.0	2.0416473682	1.4061732199	1.3387976564
C	6.0	-0.0579357226	2.2642566528	2.1800664551
C	6.0	2.7473067412	2.2776817802	2.1656671457
C	6.0	0.6458093098	3.1371431829	3.0148770145
C	6.0	2.0438755194	3.1438762803	3.0076902829
H	1.0	-1.1433206013	2.2383665078	2.1753168922
H	1.0	3.8327857110	2.2621575304	2.1497231194
H	1.0	2.5909366310	3.8225509210	3.6554476666
H	1.0	0.0989753601	3.8105412409	3.6683073322

J



E(B3LYP-PCM): S0 = –1865.313482*
E(HOMO) = –0.1753; E(LUMO) = –0.1095

E(TDDFT-B3LYP-PCM): S1 = –1865.258448
Oscillator strength S1 → S0 = 2.8581*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
161	162	-0.998664	0.099373
160	163	0.092062	0.026214
159	166	0.030600	0.013483

E(ORMAS-PT2-PCM): S0 = –1860.447761*
E(ORMAS-PT2-PCM): S1 = –1860.401257

Optimized TDDFT-B3LYP-PCM geometry:

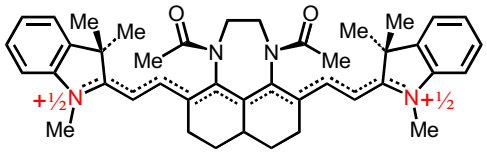
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0919821004	0.2741643288	-0.8223064528
C	6.0	-1.1278195403	0.0268523895	-1.5195443858
C	6.0	3.8465140333	0.5133755464	-1.4233693753
C	6.0	-2.3285981402	-0.0680360054	-0.8039920904
C	6.0	5.0392342170	0.2263596228	-0.7336900246
H	1.0	-2.2557623650	0.1058908138	0.2618869539
H	1.0	4.9339093309	-0.0939829864	0.2954388212
C	6.0	-3.5885384404	-0.3732626475	-1.3554494895
C	6.0	6.3276496564	0.2851374963	-1.2919413021
H	1.0	-3.6360746367	-0.5618870573	-2.4232221534
H	1.0	6.4148016602	0.6482648212	-2.3109189970
C	6.0	-4.7900805912	-0.4674498570	-0.6592711587
C	6.0	7.5177007158	-0.0858786918	-0.6675349399
N	7.0	-5.9679858533	-0.7792048788	-1.2930416305
N	7.0	8.7289039687	0.0291300770	-1.3016859409
C	6.0	-6.0810206155	-1.0447088248	-2.7214005695
C	6.0	8.8997411219	0.5531839980	-2.6509215613
H	1.0	-7.1183458816	-1.2615213331	-2.9697522645
H	1.0	9.9587818902	0.5711056665	-2.9014939551
H	1.0	-5.4640358570	-1.9064735943	-2.9969064761
H	1.0	8.3758585416	-0.0800808450	-3.3750352086
H	1.0	-5.7565369901	-0.1713292199	-3.2970325800
H	1.0	8.5060250566	1.5728745586	-2.7146737565

C	6.0	-7.0424200305	-0.8127881901	-0.3975458134
C	6.0	9.7777608021	-0.4335164128	-0.4985675399
C	6.0	-8.3906122457	-1.0894891782	-0.6460988512
C	6.0	11.1460709148	-0.4920847922	-0.7805059679
H	1.0	-8.7596741102	-1.3217944403	-1.6393088221
H	1.0	11.5564683845	-0.1574135550	-1.7271771015
C	6.0	-9.2654077186	-1.0573621610	0.4434726411
C	6.0	11.9855510470	-1.0074759719	0.2113338886
H	1.0	-10.3185817471	-1.2688332239	0.2808469780
H	1.0	13.0534629049	-1.0658831030	0.0203005909
C	6.0	-8.8095245991	-0.7598072645	1.7343680547
C	6.0	11.4757644326	-1.4472309387	1.4399253351
H	1.0	-9.5102685810	-0.7423069351	2.5640224118
H	1.0	12.1499454996	-1.8440735299	2.1934267937
C	6.0	-7.4522359134	-0.4847775237	1.9628650887
C	6.0	10.0989576910	-1.3796280884	1.7034472100
H	1.0	-7.1036243849	-0.2553862489	2.9666627960
H	1.0	9.7079518461	-1.7226541645	2.6579706259
C	6.0	-6.5713967036	-0.5118308117	0.8914107158
C	6.0	9.2527649919	-0.8713397430	0.7285356049
C	6.0	-5.0729205195	-0.2630822825	0.8360797228
C	6.0	7.7442688425	-0.6860212356	0.7270881163
C	6.0	-4.3262932695	-1.2992826937	1.7151927450
C	6.0	7.0348287512	-2.0568313454	0.8777883791
C	6.0	-4.7501162591	1.1831410238	1.2919728166
C	6.0	7.3208942311	0.2816157143	1.8619577456
H	1.0	-4.5707543834	-2.3216726862	1.4100114767
H	1.0	7.3507746086	-2.7490857268	0.0909056203
H	1.0	-5.2706481493	1.9159947241	0.6672331041
H	1.0	7.8152594019	1.2524444013	1.7568544612
H	1.0	-4.6248617397	-1.1728325453	2.7616196633
H	1.0	7.2903813523	-2.4992900765	1.8469184862
H	1.0	-5.0784522102	1.3206744418	2.3280375338
H	1.0	7.6067422593	-0.1462626648	2.8291025901
H	1.0	-3.2421094947	-1.1717953462	1.6550958191
H	1.0	5.9474437680	-1.9527358665	0.8281548663
H	1.0	-3.6775765285	1.3904758718	1.2454336024
H	1.0	6.2395069065	0.4432949821	1.8753724516
C	6.0	1.3526869280	0.3686730414	-1.4551732073
C	6.0	2.5915982083	0.4503921668	-0.7577832789
C	6.0	1.4133882580	0.3411370911	-2.9785887041
C	6.0	-1.0673702572	-0.1330628810	-3.0216970188
C	6.0	3.8878348254	0.8352722432	-2.9036827781
C	6.0	2.5340870513	1.2716598564	-3.4605284096
C	6.0	0.0686544397	0.7016963953	-3.6146301870
H	1.0	4.2393453804	-0.0547925720	-3.4471652271
H	1.0	4.6364777953	1.6156285199	-3.0920798239
H	1.0	-0.9143777889	-1.1937218037	-3.2753433068
H	1.0	-2.0180112020	0.1599426264	-3.4777340359
H	1.0	1.6699746010	-0.6867767512	-3.2875353546
H	1.0	2.5682877170	1.2757602854	-4.5563085930
H	1.0	2.3053624371	2.2975756451	-3.1412357316

H	1.0	0.1251256586	0.5471370842	-4.6984276004
H	1.0	-0.1386951994	1.7682443771	-3.4499971828
O	8.0	-0.0234855451	0.4851886503	0.5404291810
N	7.0	2.5929342186	0.2993425388	0.6665201198
C	6.0	0.4156840118	-0.5596880393	1.4216361605
C	6.0	1.9015381591	-0.8833459811	1.1885640106
C	6.0	2.8742014404	1.3210383236	1.5538956970
O	8.0	2.7490211455	1.1446167440	2.7674548745
C	6.0	3.3335818315	2.6516582713	0.9876475344
H	1.0	4.3500334814	2.5845408450	0.5865330850
H	1.0	3.3204490175	3.3831120162	1.7974981952
H	1.0	2.6814395931	2.9878350034	0.1755584407
H	1.0	2.3684975369	-1.1966325651	2.1251420877
H	1.0	2.0240183428	-1.6833857746	0.4558730369
H	1.0	0.2581433236	-0.1525322173	2.4215196836
H	1.0	-0.2027749695	-1.4580475799	1.2957154108

K



E(B3LYP-PCM): S0 = –1998.026592*
E(HOMO) = –0.1772; E(LUMO) = –0.1152

E(TDDFT-B3LYP-PCM): S1 = –1997.974183
Oscillator strength S1 → S0 = 2.7722*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
172	173	-1.000044	0.111543
171	174	-0.090379	-0.029140

E(ORMAS-PT2-PCM): S0 = –1992.837197*
E(ORMAS-PT2-PCM): S1 = –1992.792851

Optimized TDDFT-B3LYP-PCM geometry:

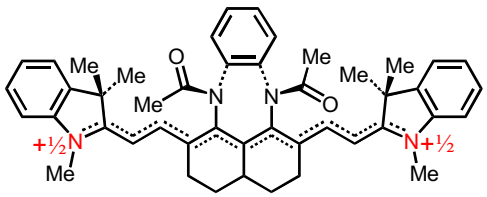
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0847639979	0.6350919345	-0.6918719676
C	6.0	-1.1721278646	0.5932316595	-1.3606310466
C	6.0	3.7986449678	0.2729255583	-1.4791553161
C	6.0	-2.3373058784	0.1972720334	-0.6798863475
C	6.0	5.0084080255	0.1137891892	-0.7847359423
H	1.0	-2.2154409122	-0.1364055638	0.3430958836
H	1.0	4.9714272291	0.2568277329	0.2879213329
C	6.0	-3.6238653368	0.1684605261	-1.2435630162
C	6.0	6.2426612652	-0.2406193940	-1.3603094436
H	1.0	-3.7329345030	0.5435799339	-2.2557196415
H	1.0	6.2773073382	-0.3665247460	-2.4373038256
C	6.0	-4.7853354408	-0.2974649626	-0.6280567981
C	6.0	7.4387662482	-0.4508635794	-0.6782902611
N	7.0	-5.9992675902	-0.2562123927	-1.2622944320
N	7.0	8.5943095170	-0.7770654188	-1.3427008779
C	6.0	-6.2046955026	0.2758150021	-2.6041644460
C	6.0	8.6912525400	-0.9235943941	-2.7899606634
H	1.0	-7.2656539103	0.2515088757	-2.8454788757
H	1.0	9.7169056141	-1.1643656683	-3.0630597005
H	1.0	-5.6591781418	-0.3247008581	-3.3399793229
H	1.0	8.0350780364	-1.7298906531	-3.1341743860
H	1.0	-5.8568509276	1.3123991848	-2.6560635586
H	1.0	8.4051084153	0.0102119810	-3.2849909708
C	6.0	-7.0160408397	-0.8008011118	-0.4680740424

C	6.0	9.6649457030	-0.9552584932	-0.4599302690
C	6.0	-8.3763091751	-0.9483302875	-0.7550955808
C	6.0	10.9938665890	-1.2900161098	-0.7392420071
H	1.0	-8.8064419955	-0.6290743918	-1.6982526374
H	1.0	11.3478644359	-1.4570728280	-1.7508301297
C	6.0	-9.1803441195	-1.5331475991	0.2274404567
C	6.0	11.8689834740	-1.4043819460	0.3442422831
H	1.0	-10.2413209377	-1.6621045251	0.0327052752
H	1.0	12.9075334643	-1.6637541032	0.1588255843
C	6.0	-8.6432942863	-1.9543509042	1.4509653191
C	6.0	11.4318333551	-1.1921098421	1.6586027487
H	1.0	-9.2902236762	-2.4062846909	2.1972352628
H	1.0	12.1330681742	-1.2872311534	2.4825082867
C	6.0	-7.2748871581	-1.7968171693	1.7193817731
C	6.0	10.0938596284	-0.8570790529	1.9176080343
H	1.0	-6.8634364157	-2.1260368795	2.6700661338
H	1.0	9.7593282823	-0.6939206257	2.9388643537
C	6.0	-6.4638766759	-1.2186025740	0.7534913312
C	6.0	9.2129086597	-0.7405417556	0.8525275700
C	6.0	-4.9718405049	-0.9299453519	0.7583983510
C	6.0	7.7327960560	-0.3972606265	0.8282253087
C	6.0	-4.1697927039	-2.2502502646	0.8976558808
C	6.0	6.9229479315	-1.4645305488	1.6092943763
C	6.0	-4.6195280319	0.0504046931	1.9071998674
C	6.0	7.4996383635	1.0152625651	1.4247769894
H	1.0	-4.4290325134	-2.9536092776	0.0999449639
H	1.0	7.0800335131	-2.4631111179	1.1895940098
H	1.0	-5.1636830202	0.9941149446	1.8012579544
H	1.0	8.0473242182	1.7764744427	0.8603006914
H	1.0	-4.4041531509	-2.7197658444	1.8590322480
H	1.0	7.2472621601	-1.4765296630	2.6554938601
H	1.0	-4.8983033907	-0.4001071660	2.8659036578
H	1.0	7.8547457453	1.0360370708	2.4607977795
H	1.0	-3.0917463363	-2.0705945488	0.8606709329
H	1.0	5.8509890102	-1.2484842195	1.5898612541
H	1.0	-3.5484108791	0.2686847250	1.9423667387
H	1.0	6.4396112751	1.2844710467	1.4306707014
C	6.0	1.3230283734	0.6060339166	-1.3957205978
C	6.0	2.6012470535	0.6186811100	-0.7802279209
C	6.0	1.2386504957	0.4912592578	-2.9135323625
C	6.0	-1.2444381893	0.9237335299	-2.8381471039
C	6.0	3.7168852612	0.0481228597	-2.9723474408
C	6.0	2.5649862966	0.8389746800	-3.5896537594
C	6.0	0.0929044330	1.3789260865	-3.4186546653
H	1.0	3.5789328222	-1.0253128707	-3.1753973442
H	1.0	4.6584858137	0.3319927967	-3.4528135240
H	1.0	-1.5933583068	0.0314094389	-3.3785602696
H	1.0	-2.0085833191	1.6939649355	-3.0076843776
H	1.0	0.9943165670	-0.5551217771	-3.1640117149
H	1.0	2.4938734750	0.6283939941	-4.6627712887
H	1.0	2.7614546557	1.9150627193	-3.4845342057
H	1.0	0.0518075173	1.3467659569	-4.5135374976

H	1.0	0.2987752784	2.4198614943	-3.1349168337
N	7.0	0.0900331260	0.5075144134	0.7309704034
N	7.0	2.7217496356	0.9366221079	0.6180367748
C	6.0	0.9038058637	-0.5787707041	1.2927255768
C	6.0	2.3217324309	-0.0702849221	1.6064298091
C	6.0	3.1639167507	2.1703914230	1.0566147999
C	6.0	-0.4348345587	1.4376226906	1.6118075822
O	8.0	3.3398832094	2.4044026879	2.2541225888
O	8.0	-0.3963403676	1.2341744652	2.8266991392
C	6.0	3.4308628326	3.2314423000	0.0027622996
C	6.0	-1.0449204948	2.7094405519	1.0521126046
H	1.0	4.3295593160	2.9903260223	-0.5748336635
H	1.0	3.5863145925	4.1816511464	0.5163996980
H	1.0	2.6015183839	3.3262988998	-0.7045942492
H	1.0	-0.5658401662	3.0450091682	0.1291966439
H	1.0	-2.1098048035	2.5637620905	0.8404192399
H	1.0	-0.9547158804	3.4815093499	1.8194088184
H	1.0	2.3492513470	0.4251013647	2.5760682367
H	1.0	3.0278094229	-0.9106746449	1.6200220391
H	1.0	0.9211558575	-1.3899331362	0.5621057157
H	1.0	0.4299551806	-0.9457924889	2.2051652105

L



E(B3LYP-PCM): S0 = –2150.353840*
E(HOMO) = –0.1773; E(LUMO) = –0.1170

E(TDDFT-B3LYP-PCM): S1 = –2150.302515
Oscillator strength S1 → S0 = 2.8182*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
182	185	-0.033777	-0.023280
184	185	1.000837	-0.117959
183	186	0.091132	0.031708

E(ORMAS-PT2-PCM): S0 = –2144.814488*
E(ORMAS-PT2-PCM): S1 = –2144.772728

Optimized TDDFT-B3LYP-PCM geometry:

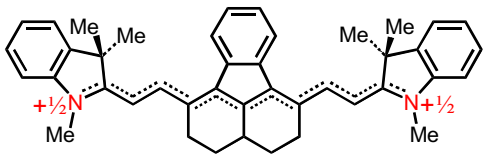
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0549676644	0.3537792534	-0.6782240250
C	6.0	-1.1770017648	0.1962531026	-1.3841461814
C	6.0	3.8283664015	0.4036597135	-1.3667821395
C	6.0	-2.3811874531	-0.0427663397	-0.7029884989
C	6.0	5.0354211488	0.1384579484	-0.6913006544
H	1.0	-2.3372379236	-0.0757462527	0.3764780450
H	1.0	4.9738684051	-0.0431923028	0.3737578635
C	6.0	-3.6262637610	-0.2633735385	-1.3195816291
C	6.0	6.2963622899	0.0679318784	-1.3085954555
H	1.0	-3.6515863521	-0.2890324272	-2.4035435361
H	1.0	6.3395396865	0.2658960578	-2.3737522736
C	6.0	-4.8473612117	-0.4506348621	-0.6747442087
C	6.0	7.5136909546	-0.2293638486	-0.6956305979
N	7.0	-6.0005418277	-0.6888390645	-1.3772346905
N	7.0	8.6853197537	-0.2420226532	-1.4062511079
C	6.0	-6.0663408509	-0.7953343289	-2.8299906357
C	6.0	8.7828854784	0.0530369878	-2.8314086107
H	1.0	-7.0816521876	-1.0475937386	-3.1300081735
H	1.0	9.8276116669	0.0329893792	-3.1350189244
H	1.0	-5.3896882696	-1.5809908790	-3.1803807671
H	1.0	8.2289896595	-0.6916505431	-3.4126437268

H	1.0	-5.7861460738	0.1559493033	-3.2952057174
H	1.0	8.3756780575	1.0478679132	-3.0371367175
C	6.0	-7.1072519639	-0.8083991487	-0.5285289850
C	6.0	9.7784086406	-0.5682095132	-0.5949965706
C	6.0	-8.4468202296	-1.0443715443	-0.8525815156
C	6.0	11.1277397423	-0.6868029996	-0.9413651058
H	1.0	-8.7821611034	-1.1643840964	-1.8771084754
H	1.0	11.4814298154	-0.5242942168	-1.9536671887
C	6.0	-9.3589948052	-1.1212809066	0.2035042927
C	6.0	12.0237507859	-1.0276090399	0.0753343634
H	1.0	-10.4070520508	-1.3035030176	-0.0170599880
H	1.0	13.0789499829	-1.1274239956	-0.1630410535
C	6.0	-8.9469063889	-0.9673873788	1.5339354789
C	6.0	11.5860193123	-1.2418692916	1.3888438025
H	1.0	-9.6770436492	-1.0313517112	2.3354564519
H	1.0	12.3036210089	-1.5055234873	2.1603167993
C	6.0	-7.5975386111	-0.7304554729	1.8379495823
C	6.0	10.2264295068	-1.1190634050	1.7155211997
H	1.0	-7.2822719944	-0.6111772225	2.8712756503
H	1.0	9.8935441378	-1.2882527837	2.7362606936
C	6.0	-6.6803691202	-0.6511349927	0.8002709994
C	6.0	9.3242202211	-0.7816230439	0.7167482003
C	6.0	-5.1807409184	-0.4076505670	0.8228505606
C	6.0	7.8170734396	-0.5907927150	0.7646528240
C	6.0	-4.4714705735	-1.5365595993	1.6135651878
C	6.0	7.1240728996	-1.9162293599	1.1739735092
C	6.0	-4.8690216323	0.9829228688	1.4353006563
C	6.0	7.4465927028	0.5516725749	1.7446599033
H	1.0	-4.6722759622	-2.5160604123	1.1686979966
H	1.0	7.4175624412	-2.7356186623	0.5103204856
H	1.0	-5.4105131910	1.7724784124	0.9043936804
H	1.0	7.9001051299	1.4986583809	1.4359011177
H	1.0	-4.8371788771	-1.5453616635	2.6458682964
H	1.0	7.4120370230	-2.1806456510	2.1969802442
H	1.0	-5.1826888659	0.9993169943	2.4847553423
H	1.0	7.8145004456	0.3048815023	2.7462151892
H	1.0	-3.3882940160	-1.3892960278	1.6439249708
H	1.0	6.0350710367	-1.8231291826	1.1375850206
H	1.0	-3.8011872815	1.2160573647	1.3924952148
H	1.0	6.3642264738	0.6931872145	1.8132994722
C	6.0	1.3179411838	0.4433178428	-1.3223881849
C	6.0	2.5873869212	0.4713987646	-0.6670902075
C	6.0	1.3342088711	0.4423072190	-2.8510392824
C	6.0	-1.1726855595	0.2668560184	-2.8954627207
C	6.0	3.8429486928	0.5886276509	-2.8687373700
C	6.0	2.5494624110	1.2033312416	-3.3846317548
C	6.0	0.0402315718	1.0198055810	-3.4246678714
H	1.0	4.0071037396	-0.3870073010	-3.3511809752
H	1.0	4.6925068552	1.2177656056	-3.1580807335
H	1.0	-1.1798940802	-0.7551507226	-3.3063148656
H	1.0	-2.0895233025	0.7472993840	-3.2522733931
H	1.0	1.4155861221	-0.6061227605	-3.1864931521

H	1.0	2.5388641591	1.1900487385	-4.4804500456
H	1.0	2.4826426710	2.2548523130	-3.0734850842
H	1.0	0.0701024137	0.9644435542	-4.5189266649
H	1.0	-0.0344209883	2.0821846648	-3.1555548245
N	7.0	-0.0149198949	0.3193000572	0.7650094823
N	7.0	2.6602773198	0.4600330643	0.7725760540
C	6.0	0.6839494843	-0.7564674522	1.4077988506
C	6.0	2.0804401668	-0.6752646221	1.4318416351
C	6.0	0.0343244255	-1.8609860003	1.9617951866
C	6.0	2.8335692698	-1.6791128342	2.0390489507
C	6.0	0.7877138846	-2.8656651341	2.5732735584
C	6.0	2.1821689787	-2.7717153661	2.6168078565
H	1.0	-1.0482166842	-1.9311520514	1.9173387327
H	1.0	3.9154077800	-1.6028784749	2.0696555112
H	1.0	2.7658029161	-3.5535225424	3.0940154359
H	1.0	0.2856881057	-3.7228552116	3.0123288864
C	6.0	3.0650989383	1.5432107678	1.5428682588
C	6.0	-0.5152634095	1.4104381307	1.4694523838
O	8.0	3.0857930177	1.4629744861	2.7700701132
O	8.0	-0.9966594706	2.3770183677	0.8855631897
C	6.0	3.4653307968	2.8108225604	0.8144496175
C	6.0	-0.4482849818	1.3321518061	2.9841356625
H	1.0	4.4528847559	2.7034361961	0.3535491129
H	1.0	3.5061361611	3.6176026868	1.5483083939
H	1.0	2.7573808505	3.0661068907	0.0205613105
H	1.0	0.5891824246	1.2573624549	3.3265014625
H	1.0	-0.8991017408	2.2410364066	3.3861004297
H	1.0	-0.9870494689	0.4609757377	3.3704825343

M



E(B3LYP-PCM): S0 = –1734.576100*
E(HOMO) = –0.1717; E(LUMO) = –0.1200

E(TDDFT-B3LYP-PCM): S1 = –1734.533586
Oscillator strength S1 → S0 = 1.8389*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
151	155	-0.055672	-0.025544
152	155	-0.097302	0.004387
154	155	-0.999548	0.141609
153	156	0.071797	0.034445
152	157	-0.049266	-0.012406

E(ORMAS-PT2-PCM): S0 = –1730.004146*
E(ORMAS-PT2-PCM): S1 = –1729.961713

Optimized TDDFT-B3LYP-PCM geometry:

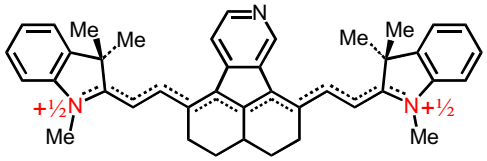
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0915050175	1.1750997992	-1.1853520063
C	6.0	-1.1492447770	0.6609601771	-1.6495649810
C	6.0	3.7118627504	1.3590520268	-1.8325585342
C	6.0	-2.2481704827	0.4622563223	-0.8031513502
C	6.0	4.8842030508	1.5239886906	-1.0821424288
H	1.0	-2.1074919804	0.6954068669	0.2438217354
H	1.0	4.7650147368	1.7615851245	-0.0340686662
C	6.0	-3.4858584621	-0.0797895834	-1.1987155450
C	6.0	6.1917607823	1.3416274090	-1.5712720308
H	1.0	-3.6142498738	-0.3050917478	-2.2518581184
H	1.0	6.2981819770	1.0925276199	-2.6213023805
C	6.0	-4.5665541133	-0.3770151214	-0.3723775875
C	6.0	7.3732918949	1.4348716499	-0.8395145528
N	7.0	-5.7266673534	-0.9066620160	-0.8735581284
N	7.0	8.5952834465	1.2218633662	-1.4207230072
C	6.0	-5.9552791344	-1.1892082665	-2.2852073798
C	6.0	8.7842622123	0.8755933236	-2.8243296843
H	1.0	-6.9801102034	-1.5282738621	-2.4251165871
H	1.0	9.8433177159	0.7173160818	-3.0190520501
H	1.0	-5.2719931659	-1.9707720252	-2.6349387766
H	1.0	8.2412554200	-0.0449009294	-3.0611941742

H	1.0	-5.8015469872	-0.2838752566	-2.8805549869
H	1.0	8.4220254775	1.6836359614	-3.4686355362
C	6.0	-6.6587756702	-1.1652180524	0.1416185874
C	6.0	9.6406478540	1.3704111137	-0.4977240751
C	6.0	-7.9391609538	-1.7157718447	0.0441087929
C	6.0	11.0177163539	1.2427172907	-0.6964316508
H	1.0	-8.3675849716	-2.0203704585	-0.9047338025
H	1.0	11.4427443355	0.9979520247	-1.6639199874
C	6.0	-8.6652967744	-1.8694684448	1.2294453844
C	6.0	11.8485473561	1.4455526653	0.4100798501
H	1.0	-9.6630192157	-2.2968737937	1.1842684674
H	1.0	12.9238358179	1.3528758096	0.2858220624
C	6.0	-8.1296817397	-1.4858036719	2.4651125560
C	6.0	11.3205670074	1.7638935209	1.6673915372
H	1.0	-8.7141848441	-1.6151816380	3.3713449334
H	1.0	11.9876815078	1.9160996535	2.5108751688
C	6.0	-6.8411743850	-0.9351955053	2.5407717875
C	6.0	9.9340732894	1.8888058575	1.8448354269
H	1.0	-6.4281282001	-0.6405436381	3.5021326156
H	1.0	9.5285253781	2.1369050409	2.8223533786
C	6.0	-6.1083163000	-0.7790811922	1.3728576665
C	6.0	9.0975003976	1.6909793742	0.7556810421
C	6.0	-4.7114673367	-0.2217924629	1.1489555220
C	6.0	7.5832765892	1.7638907558	0.6458910617
C	6.0	-3.6653989601	-1.0626112082	1.9232747168
C	6.0	6.9253100570	0.7098578975	1.5725083794
C	6.0	-4.6580276691	1.2658768162	1.5812570841
C	6.0	7.0917745132	3.1924979360	0.9930684833
H	1.0	-3.6811972281	-2.1072708485	1.5967640921
H	1.0	7.2681738006	-0.2995775486	1.3242335921
H	1.0	-5.3992447739	1.8600520688	1.0375793266
H	1.0	7.5624233166	3.9386011586	0.3450726885
H	1.0	-3.8944068992	-1.0345605666	2.9939829904
H	1.0	7.1972056613	0.9187086536	2.6127991961
H	1.0	-4.8743339815	1.3423466324	2.6521801908
H	1.0	7.3495932186	3.4271029047	2.0313022379
H	1.0	-2.6522161309	-0.6748665095	1.7858073757
H	1.0	5.8345969296	0.7296584978	1.4973559789
H	1.0	-3.6711310070	1.7025995290	1.4035410406
H	1.0	6.0071806564	3.2825893721	0.8859107944
C	6.0	1.2690279363	1.0383576476	-1.9681227793
C	6.0	2.4151302950	1.5082841467	-1.2713399812
C	6.0	1.2943504688	0.4759258671	-3.3481810900
C	6.0	-1.2160827938	0.2143990347	-3.1084148475
C	6.0	3.7934529647	0.8994378354	-3.2866070781
C	6.0	2.4950706803	1.0816339564	-4.0899939791
C	6.0	-0.0743353001	0.7420441431	-3.9923693088
H	1.0	4.0827546755	-0.1631017510	-3.3048734059
H	1.0	4.6008380706	1.4380758616	-3.7960064802
H	1.0	-1.2200840440	-0.8863741155	-3.1406118852
H	1.0	-2.1726078919	0.5282358061	-3.5430636836
H	1.0	1.4421661560	-0.6179855851	-3.2907941689

H	1.0	2.6092352228	0.6190149206	-5.0772329369
H	1.0	2.3100920186	2.1523995343	-4.2521366871
H	1.0	-0.1327340284	0.2741561917	-4.9821328686
H	1.0	-0.1915585333	1.8246275311	-4.1385353754
C	6.0	1.9238349761	2.0511186912	0.0000317991
C	6.0	0.4999809377	1.8463493337	0.0515054035
C	6.0	2.5567612939	2.7515602088	1.0344370393
C	6.0	1.8088886472	3.2194571441	2.1181592282
C	6.0	-0.2347337227	2.3524759888	1.1303515267
C	6.0	0.4221318779	3.0221344275	2.1657670769
H	1.0	2.3063794216	3.7608266384	2.9182638676
H	1.0	3.6173407097	2.9738989002	0.9990595802
H	1.0	-0.1521607062	3.4106279839	3.0023258918
H	1.0	-1.3153359494	2.2682524279	1.1645446668

N



E(B3LYP-PCM): S0 = –1750.613644*
E(HOMO) = –0.1741; E(LUMO) = –0.1242

E(TDDFT-B3LYP-PCM): S1 = –1750.571824
Oscillator strength S1 → S0 = 1.9524*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
151	155	-0.053458	-0.020656
152	155	-0.045098	0.012923
154	155	-1.004454	0.151525
153	156	-0.072918	-0.036212
152	157	-0.048300	-0.016335

E(ORMAS-PT2-PCM): S0 = –1746.033925*
E(ORMAS-PT2-PCM): S1 = –1745.991432

Optimized TDDFT-B3LYP-PCM geometry:

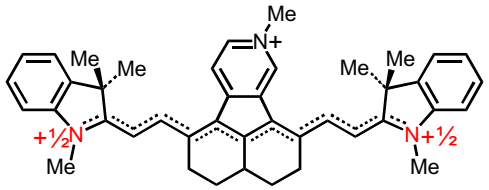
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.1066173127	1.0845231574	-1.1609162509
C	6.0	-1.1437878232	0.5973432030	-1.6361907079
C	6.0	3.7200390250	1.3195552794	-1.8263626669
C	6.0	-2.2486966710	0.4139826617	-0.7964976503
C	6.0	4.8963650988	1.5008053544	-1.0815881934
H	1.0	-2.1136363012	0.6500503882	0.2502548874
H	1.0	4.7795392816	1.7302917952	-0.0314089001
C	6.0	-3.4907103591	-0.1131004663	-1.1988592907
C	6.0	6.2008765279	1.3469680962	-1.5798746569
H	1.0	-3.6112084099	-0.3525473268	-2.2496850166
H	1.0	6.3065651301	1.1043252529	-2.6313704725
C	6.0	-4.5846142273	-0.3808006063	-0.3792361807
C	6.0	7.3857500263	1.4602000964	-0.8516137167
N	7.0	-5.7441282231	-0.9059828875	-0.8841887197
N	7.0	8.6059395743	1.2711576135	-1.4386191701
C	6.0	-5.9577592938	-1.2176871716	-2.2924696459
C	6.0	8.7957942221	0.9309315407	-2.8446001193
H	1.0	-6.9801862249	-1.5620567225	-2.4358504096
H	1.0	9.8561934348	0.7861450235	-3.0417296317
H	1.0	-5.2695081564	-2.0050492767	-2.6180377216

H	1.0	8.2636900888	0.0044378682	-3.0814329262
H	1.0	-5.7995453969	-0.3244263792	-2.9047464657
H	1.0	8.4222153505	1.7366259091	-3.4850230205
C	6.0	-6.6950656941	-1.1240433999	0.1222154231
C	6.0	9.6539157890	1.4361345822	-0.5203479675
C	6.0	-7.9827261104	-1.6566804846	0.0176953292
C	6.0	11.0318078933	1.3320186730	-0.7267330189
H	1.0	-8.4015634542	-1.9775650257	-0.9299797603
H	1.0	11.4561724585	1.0970148915	-1.6968414647
C	6.0	-8.7288460331	-1.7690454276	1.1946835348
C	6.0	11.8638672893	1.5457247220	0.3764159320
H	1.0	-9.7326650096	-2.1812155638	1.1449068923
H	1.0	12.9399441471	1.4713715225	0.2474924564
C	6.0	-8.2052367666	-1.3634092268	2.4289220223
C	6.0	11.3359278769	1.8519256882	1.6371050544
H	1.0	-8.8056121013	-1.4611797992	3.3286885662
H	1.0	12.0044502986	2.0129311860	2.4777928505
C	6.0	-6.9094366791	-0.8315545568	2.5118971034
C	6.0	9.9487280821	1.9532762404	1.8220054755
H	1.0	-6.5070512362	-0.5195509082	3.4722318746
H	1.0	9.5439963775	2.1918627307	2.8021247445
C	6.0	-6.1565150663	-0.7158204123	1.3520692578
C	6.0	9.1107686221	1.7441790391	0.7360010238
C	6.0	-4.7484589177	-0.1850608158	1.1351433011
C	6.0	7.5955196250	1.7896917982	0.6331269306
C	6.0	-3.7268406077	-1.0199034765	1.9479067312
C	6.0	6.9617776318	0.7211912965	1.5604361555
C	6.0	-4.6800057626	1.3133396189	1.5261726849
C	6.0	7.0785071901	3.2084743840	0.9847688856
H	1.0	-3.7454480276	-2.0706601919	1.6420288589
H	1.0	7.3202832391	-0.2814273506	1.3069784409
H	1.0	-5.4119607150	1.9002893117	0.9624864910
H	1.0	7.5325995271	3.9644947448	0.3365580285
H	1.0	-3.9787233288	-0.9679090703	3.0124574441
H	1.0	7.2370506223	0.9321896834	2.5992939951
H	1.0	-4.8998791890	1.4230428537	2.5934817015
H	1.0	7.3364099701	3.4451497151	2.0223874996
H	1.0	-2.7070652031	-0.6445646758	1.8256138095
H	1.0	5.8704298558	0.7222454231	1.4928288522
H	1.0	-3.6877273337	1.7344779355	1.3398477349
H	1.0	5.9920054598	3.2782243791	0.8821874881
C	6.0	1.2781071752	0.9754407030	-1.9506428398
C	6.0	2.4289793962	1.4346425100	-1.2511725511
C	6.0	1.2987161691	0.4515674980	-3.3467779083
C	6.0	-1.2100596606	0.1752235177	-3.1011735230
C	6.0	3.7960965880	0.8844358837	-3.2871089005
C	6.0	2.4928676054	1.0808028179	-4.0792555622
C	6.0	-0.0741444890	0.7281249890	-3.9775492035
H	1.0	4.0853323847	-0.1776500949	-3.3229478742
H	1.0	4.6006895059	1.4316463804	-3.7911660623
H	1.0	-1.2027949382	-0.9249938635	-3.1508795136
H	1.0	-2.1699271458	0.4869398792	-3.5289303963

H	1.0	1.4515447885	-0.6424421060	-3.3176683766
H	1.0	2.6037369119	0.6432301619	-5.0780275061
H	1.0	2.3036237181	2.1546226178	-4.2135481285
H	1.0	-0.1353603184	0.2832896319	-4.9775069728
H	1.0	-0.1966302215	1.8133037363	-4.0974129546
C	6.0	1.9409918225	1.9274670497	0.0403119025
C	6.0	0.5218524353	1.7110156997	0.0965355967
C	6.0	2.5497943159	2.5958901290	1.1056613395
N	7.0	1.8860486181	3.0127412522	2.1949080097
C	6.0	-0.1681330055	2.1702979011	1.2210976344
C	6.0	0.5596632933	2.7934445986	2.2371113297
H	1.0	3.6088237596	2.8403664168	1.0922910166
H	1.0	0.0448067181	3.1493360859	3.1278593482
H	1.0	-1.2439470521	2.0894753978	1.3244749403

O



E(B3LYP-PCM): S0 = –1790.347252*
E(HOMO) = –0.1807; E(LUMO) = –0.1386

E(TDDFT-B3LYP-PCM): S1 = –1790.311710
Oscillator strength S1 → S0 = 1.5632*

OCC I	VIR A	EXCITATION AMPLITUDE X(I->A)	DE-EXCITATION AMPLITUDE Y(A->I)
152	159	0.042263	0.012341
153	159	0.034882	0.010552
158	159	-1.012090	0.188536
156	160	-0.034776	-0.012894
158	160	0.043640	0.011549
157	161	-0.063279	-0.038103

E(ORMAS-PT2-PCM): S0 = –1785.646175*
E(ORMAS-PT2-PCM): S1 = –1785.609347

Optimized TDDFT-B3LYP-PCM geometry:

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	0.0856031484	1.1833885991	-1.1898342607
C	6.0	-1.1592101378	0.6650397529	-1.6539647943
C	6.0	3.7086593018	1.3715356840	-1.8283487424
C	6.0	-2.2507305761	0.4638043936	-0.8009485099
C	6.0	4.8783703628	1.5353821832	-1.0657879439
H	1.0	-2.1055859985	0.6872657124	0.2480453291
H	1.0	4.7555581906	1.7656770532	-0.0153383176
C	6.0	-3.4888008716	-0.0686726042	-1.1984076842
C	6.0	6.1787954860	1.3497351139	-1.5531267857
H	1.0	-3.6248721297	-0.2730890900	-2.2544647250
H	1.0	6.2849922584	1.1132775682	-2.6055707300
C	6.0	-4.5655693411	-0.3810712526	-0.3669239496
C	6.0	7.3664639947	1.4237467260	-0.8165543629
N	7.0	-5.7267488988	-0.8897636610	-0.8712425025
N	7.0	8.5769437882	1.2090707512	-1.4011086153
C	6.0	-5.9735888490	-1.1269662921	-2.2909327630
C	6.0	8.7654048780	0.8806405871	-2.8123757939
H	1.0	-6.9999895297	-1.4613262439	-2.4274817904

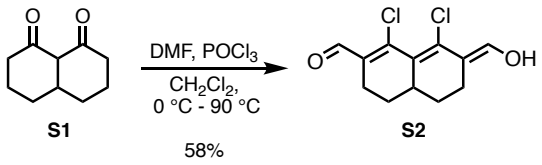
H	1.0	9.8223477325	0.7083739437	-3.0040609011
H	1.0	-5.2946809130	-1.8974591099	-2.6701992110
H	1.0	8.2089949646	-0.0274979096	-3.0614672862
H	1.0	-5.8265214156	-0.2015784437	-2.8550303009
H	1.0	8.4192543163	1.7063140532	-3.4417132944
C	6.0	-6.6533188378	-1.1725377170	0.1442498436
C	6.0	9.6289169275	1.3379934862	-0.4786692387
C	6.0	-7.9380342194	-1.7116775372	0.0392281783
C	6.0	11.0034558323	1.2016007107	-0.6865192758
H	1.0	-8.3761507069	-1.9851792190	-0.9143872300
H	1.0	11.4230129889	0.9655390601	-1.6582388477
C	6.0	-8.6541077941	-1.8941819124	1.2253283003
C	6.0	11.8379133026	1.3847356197	0.4194290368
H	1.0	-9.6550754345	-2.3130183934	1.1778987381
H	1.0	12.9120088020	1.2857841345	0.2922846881
C	6.0	-8.1042040580	-1.5486255028	2.4671083988
C	6.0	11.3143675613	1.6918676005	1.6824285790
H	1.0	-8.6826152191	-1.6999284880	3.3737125165
H	1.0	11.9857369756	1.8286575180	2.5250278124
C	6.0	-6.8120422176	-1.0092751856	2.5499441023
C	6.0	9.9305621916	1.8255390476	1.8684454512
H	1.0	-6.3899062867	-0.7450472849	3.5158631357
H	1.0	9.5311513561	2.0646423808	2.8503861066
C	6.0	-6.0885967192	-0.8250441638	1.3803642162
C	6.0	9.0900896629	1.6468733786	0.7788158321
C	6.0	-4.6914122135	-0.2720093041	1.1587043121
C	6.0	7.5780262322	1.7307763332	0.6710309789
C	6.0	-3.6423966322	-1.1485912063	1.8889175764
C	6.0	6.9135340123	0.6651743158	1.5801227709
C	6.0	-4.6216225852	1.2003689518	1.6393439113
C	6.0	7.0961794951	3.1588094970	1.0331197902
H	1.0	-3.6797022416	-2.1833610579	1.5345660898
H	1.0	7.2592905390	-0.3407924442	1.3229944120
H	1.0	-5.3579737449	1.8203905234	1.1189147796
H	1.0	7.5754267822	3.9098096636	0.3977621469
H	1.0	-3.8508412076	-1.1456085292	2.9639023918
H	1.0	7.1778985131	0.8638848037	2.6239542914
H	1.0	-4.8329576043	1.2414380789	2.7128053374
H	1.0	7.3475216023	3.3772012325	2.0760139715
H	1.0	-2.6269609072	-0.7708460753	1.7413508454
H	1.0	5.8236260230	0.6841656738	1.4968003003
H	1.0	-3.6309382983	1.6331343968	1.4744891794
H	1.0	6.0132831929	3.2583858150	0.9185040044
C	6.0	1.2671186018	1.0436613193	-1.9646382562
C	6.0	2.4109785244	1.5272584732	-1.2796674736
C	6.0	1.2945811146	0.4691670479	-3.3397442815
C	6.0	-1.2218946291	0.2209283406	-3.1109077941
C	6.0	3.7954903084	0.8984176223	-3.2752272878
C	6.0	2.4984896972	1.0660179419	-4.0838514716
C	6.0	-0.0716232118	0.7383988175	-3.9900184205
H	1.0	4.0922570310	-0.1618443402	-3.2781388640
H	1.0	4.6008711032	1.4373440097	-3.7868048400

H	1.0	-1.2352060678	-0.8796645729	-3.1394000987
H	1.0	-2.1740197636	0.5420037552	-3.5494479347
H	1.0	1.4364231031	-0.6235344099	-3.2667366613
H	1.0	2.6173970108	0.5879030271	-5.0623648854
H	1.0	2.3131333821	2.1334973265	-4.2636981330
H	1.0	-0.1268515453	0.2635800194	-4.9759594693
H	1.0	-0.1829744832	1.8200616205	-4.1445401501
C	6.0	1.9071965230	2.0887412936	-0.0249307814
C	6.0	0.4749273917	1.8709688558	0.0243067783
C	6.0	2.5062462943	2.8224301686	0.9751615243
N	7.0	1.7766078407	3.3054832297	2.0171481038
C	6.0	-0.2418636849	2.4088567990	1.0997147450
C	6.0	0.4287627417	3.1052817933	2.0855317857
H	1.0	3.5543726607	3.0881471530	0.9901913476
H	1.0	-0.0736545678	3.5374752814	2.9406165441
H	1.0	-1.3184524720	2.3350522707	1.1822192117
C	6.0	2.4652778769	4.0371997943	3.0993640190
H	1.0	3.1852975842	4.7323412384	2.6645691292
H	1.0	2.9787158591	3.3275436144	3.7532644751
H	1.0	1.7267765200	4.5961844736	

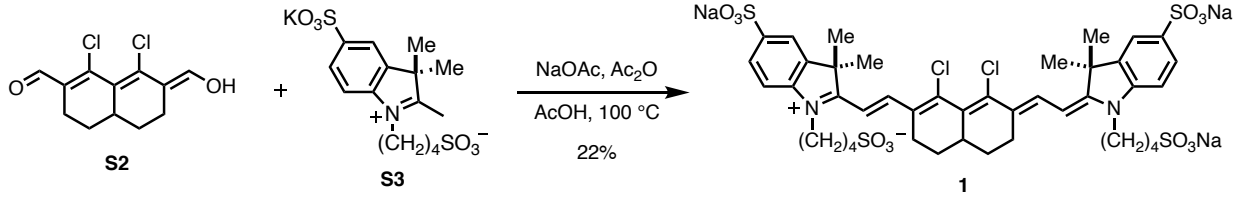
Supplementary Note 2: Synthesis and Characterization of Novel Compounds

General Materials and Methods. Unless stated otherwise, reactions were conducted in oven-dried glassware under an atmosphere of nitrogen or argon using anhydrous solvents (passed through activated alumina columns). All commercially obtained reagents were used as received. Decahydronaphthalene-1,8-dione **1** purchased from Enamine LLC (Monmouth Jct., NJ), 3,4-Dihydroxy benzoic acid, bis (pinacol) diborane, β-Alanine t-butyl ester hydrochloride and 1,3-propanesultone were purchased from Sigma-Aldrich (St. Louis, MO), and 3,4-dibromobenzoic was purchased from Combi-Blocks (San Diego, CA). Flash column chromatography was performed using reversed phase (100 Å, 20-40 micron particle size, RediSep® Rf Gold® Reversed-phase C18 or C18Aq) and silica on a CombiFlash® Rf 200i (Teledyne Isco, Inc.). High-resolution LC/MS analyses were conducted on a Thermo-Fisher LTQ-Orbitrap-XL hybrid mass spectrometer system with an Ion MAX API electrospray ion source in positive or negative ion mode. Analytical LC/MS was performed using a Shimadzu LCMS-2020 Single Quadrupole utilizing a Kinetex 2.6 µm C18 100 Å (2.1 x 50 mm) column obtained from Phenomenex, Inc. Runs employed a gradient of 0→90% MeCN/0.1% aqueous formic acid over 4.5 min at a flow rate of 0.2 mL/min. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker spectrometers (at 400 or 500 MHz or at 100 or 125 MHz) and are reported relative to deuterated solvent signals. Data for ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz), and integration. Data for ^{13}C NMR spectra are reported in terms of chemical shift. See JOC Standard Abbreviations and Acronyms for abbreviations (http://pubs.acs.org/userimages/ContentEditor/1218717864819/joceah_abbreviations.pdf).

Synthetic Procedures



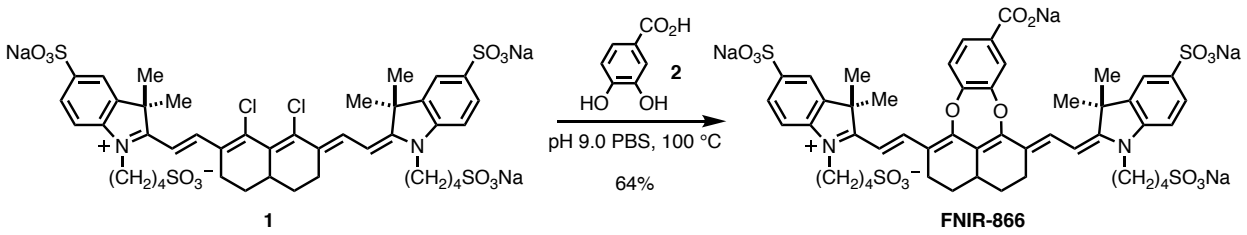
(S2): To a microwave reaction vial equipped with a magnetic stir bar was added DMF (5.0 mL, 64 mmol, 5.4 eq) and CH_2Cl_2 (2.0 mL). The vessel was sealed under argon and cooled to 0 °C, after which $POCl_3$ (9.5 mL, 100 mmol, 8.0 eq) was slowly added and stirred at 0 °C for 30 min. Decahydronaphthalene-1,8-dione **S1** (2.1 g, 13 mmol, 1.0 eq)[27] dissolved in CH_2Cl_2 (2.0 mL) was added dropwise, the ice bath was removed, and the reaction mixture was heated to 90 °C for 1 h. The reaction mixture was allowed to cool, poured onto crushed ice and the product extracted with CH_2Cl_2 (3 x 100 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure to yield **S2** (1.9 g, 58% yield) as a thick orange liquid, which was used in the next step without further purification.



(1): To a microwave reaction vial equipped with a magnetic stir bar was added bis sulfonated Indolenine **S3** (4.8 g, 12 mmol, 3.0 eq), compound S**2** (1.0 g, 3.9 mmol, 1.0 eq) and sodium acetate (1.27 g, 15.5 mmol, 4.00 eq) and the vial was sealed and flushed with argon. Acetic acid (7.6 mL, 130 mmol, 34 eq) and acetic anhydride (7.7 mL, 81 mmol, 21 eq) were added in succession under argon. The brown solution was heated to 90 °C for 30 minutes. The reaction mixture was cooled,

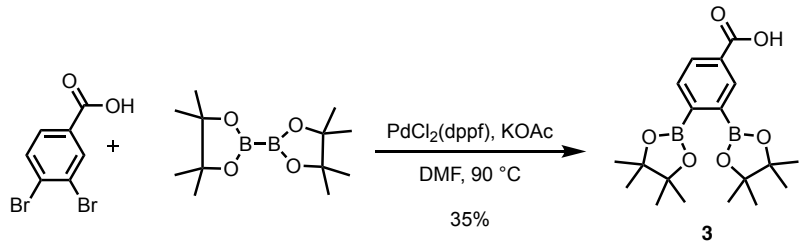
[27] Hill, C. L.; McGrath, M.; Hunt, T.; Grogan, G., A Generic and Reproducible Route to Homo-and Heteroannular Bicyclic β-Diketones via Knochel-Type 1, 4-Conjugate Additions to α, β-Unsaturated Cycloalkenones. *Synlett* **2006,** *2006* (02), 309-311.

diluted with saturated aqueous $NaHCO_3$ (5.0 mL) and directly purified by reversed-phase chromatography (150 g C_{18}Aq, 0→30% MeCN/water). The product-containing fractions were combined and lyophilized to afford **1** (910 mg, 22% yield) as a green solid. ^{1}H NMR (500 MHz, CD_3OD) δ 8.39 (d, 2H), 7.94 – 7.91 (m, 4H), 7.43 (d, 2H), 6.44 (d, 2H), 4.25 (s, 4H), 3.02 – 2.98 (m, 2H), 2.92 (t, 5H), 2.56 – 2.53 (dd, 2H), 2.23 (s, 2H), 2.03 – 1.98 (m, 10H), 1.78 (s, 12H) ppm; ^{13}C NMR (125 MHz, CD_3OD) δ 172.05, 143.72, 143.28, 141.99, 141.79, 141.23, 131.64, 130.47, 126.81, 120.00, 110.38, 103.05, 50.30, 49.16, 44.08, 40.78, 29.21, 26.71, 25.84, 25.37, 22.18 ppm; HRMS (ESI) calculated for $C_{42}H_{47}Cl_2N_2O_{12}S_4^{3-}$ (M) 969.14, observed 973.1(M+4H).

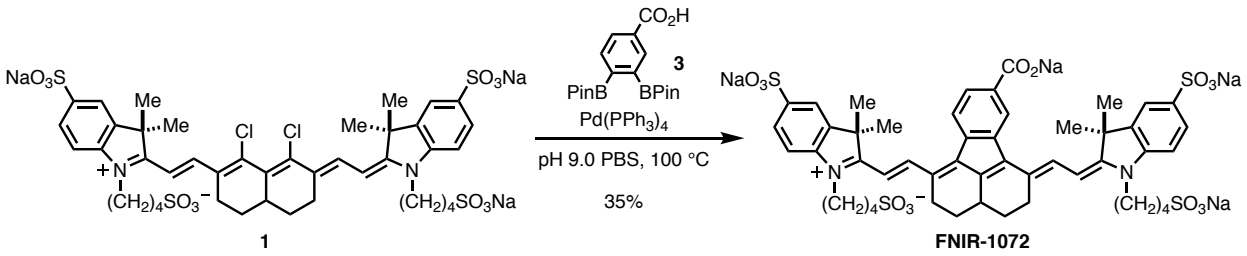


(FNIR-866): To a microwave vial equipped with a magnetic stir bar was added compound **1** (190 mg, 0.18 mmol) and 3,4-Dihydroxy benzoic acid (**2**) (140 mg, 0.90 mmol, 5.0 eq) and the vial was sealed and flushed with argon. PBS (250 mM, pH 9.0) (4.0 mL) was added and the reaction was heated to 100 °C for 18 hr. The reaction was cooled and diluted with saturated aqueous $NaHCO_3$ (3.0 mL), and the solution was directly purified by reversed-phase chromatography (50 g C_{18}Aq , 0→40% MeCN/water). The product-containing fractions were combined and lyophilized to afford **FNIR-866** (130 mg, 64% yield) as a blue solid. ^{1}H NMR (500 MHz, CD_3OD) δ 8.62 – 8.59 (d, 1H), 8.52 – 8.49 (d, 1H), 7.83 – 7.75 (m, 6H), 7.26 – 7.20 (dd, 2H), 7.12 – 7.10 (d, 1H), 6.20 – 6.12 (dd, 2H), 4.10 – 4.03 (m, 4H), 2.85 – 2.78 (m, 7H), 2.51 (s, 1H), 2.40 – 2.31 (m, 2H), 2.02 – 1.99 (m, 2H), 1.92 – 1.89 (m, 8H), 1.88 – 1.72 (m, 13H) ppm; ^{13}C NMR (125 MHz, CD_3OD) δ 171.91, 171.49, 170.66, 162.72, 162.22, 151.20, 148.97, 144.00, 143.79, 141.54, 141.10, 140.94,

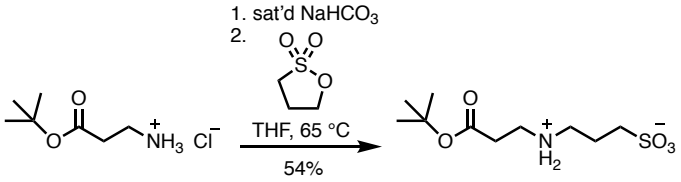
140.91, 140.60, 139.58, 127.03, 126.75, 126.72, 123.44, 123.30, 121.48, 119.99, 119.94, 119.44, 113.10, 109.90, 109.51, 100.71, 99.97, 50.42, 50.38, 43.61, 43.40, 36.95, 28.86, 27.18, 27.16, 27.14, 27.09, 25.67, 25.60, 23.85, 23.61, 22.25 ppm; HRMS (ESI) calculated for $C_{49}H_{51}N_2O_{16}S_4^{3-}$ (M) 1051.21, observed 526.1$(M+H)^{-2}$, 350.4$(M+H)^{-3}$.



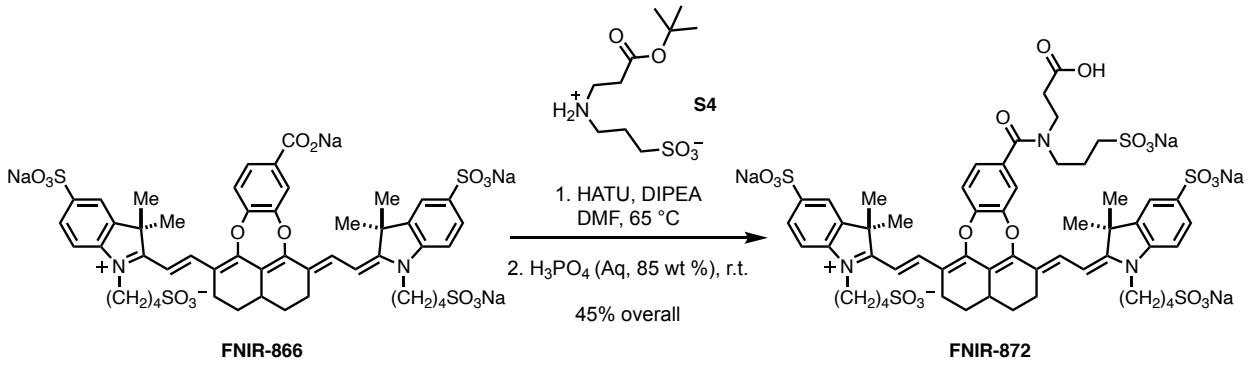
(3): To a microwave vial equipped with a magnetic stir bar was added 3,4-dibromobenzoic acid (500 mg, 1.8 mmol, 1eq), bis(pinacolato)diboron (4.53 g, 17.9 mmol, 10.0 eq) potassium acetate (1.75 g, 17.9 mmol, 10.0 eq) and [1,1'-Bis(diphenylphosphino)ferrocene]palladium(II) dichloride [$PdCl_2$(dppf)] (130 mg, 0.0017 mmol, 10 mol%). The vessel was sealed and flushed with argon. DMF (15 mL) was added and the reaction was heated to 90 °C for 24 h. The solvent was evaporated under reduced pressure and partitioned between ethyl acetate (50 mL) and water (50 mL). The aqueous layer was extracted with ethyl acetate (3 x 50 mL) and the combined organic layers were washed with water, dried over Na_2SO_4 and concentrated under reduced pressure. The resulting residue was purified by normal phase chromatography (silica 0→50% ethyl acetate/hexane), and the solvent removed to afford **3** (230 mg, 35% yield) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (m, 1H), 8.01 (d, 1H), 7.67 – 7.65 (dd, 1H), 1.32 – 1.31 (d, 24H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.24, 135.03, 133.37, 130.56, 129.35, 84.34, 83.27, 24.92 ppm; LCMS calculated for $C_{19}H_{28}B_2O_6$ (M) 374.21, observed 375.0 (M+H).



(FNIR-1072): To a microwave vial equipped with a magnetic stir bar was added Compound **1** (110 mg, 0.105 mmol, 1 eq), **3** (198 mg, 0.52 mmol, 5 eq) and $Pd(PPh_3)_4$ (12.24 mg, 0.01 mmol, 0.1 eq). The vessel was sealed and flushed with argon. PBS (250 mM, pH 9.0) (1.0 mL) was added and the reaction mixture was heated to 100 °C for 18 h. The reaction was cooled and diluted with saturated aqueous $NaHCO_3$ (2 mL) and filtered through a pad of celite. The filtrate was directly purified by reversed-phase chromatography (50 g C_{18}Aq , 0→40% MeCN/water). The product-containing fractions were combined and lyophilized to afford **FNIR-1072** (41 mg, 35% yield) as a red solid. ^{1}H NMR (400 MHz, CD_3OD) δ 8.78 – 8.75 (d, 1H), 8.62 – 8.61 (d, 1H), 8.37 – 8.34 (d, 1H), 8.05 – 8.01 (m, 2H), 7.97 – 7.92 (m, 3H), 7.84 – 7.82 (d, 1H), 7.53 – 7.51 (d, 1H), 7.33 – 7.31 (d, 1H), 6.74 – 6.70 (d, 1H), 6.47 – 6.43 (d, 1H), 4.37 – 4.33 (dd, 2H), 4.21 – 4.17 (t, 2H), 3.24 – 3.21 (d, 1H), 2.97 – 2.93 (m, 4H), 2.72 – 2.61 (m, 3H), 2.32 – 2.28 (t, 2H), 2.05 – 1.97 (m, 12H), 1.91 – 1.83 (m, 9H), 1.46 (s, 2H) ppm; ^{13}C NMR (125 MHz, CD_3OD) δ 172.68, 169.03, 146.29, 145.54, 144.03, 143.62, 143.47, 142.60, 141.79, 141.21, 140.88, 140.78, 139.95, 138.72, 136.41, 132.68, 131.46, 129.44, 126.91, 126.77, 123.38, 121.85, 119.99, 119.94, 110.98, 109.69, 104.89, 102.25, 50.43, 50.30, 49.50, 44.27, 43.59, 33.33, 29.61 - 29.46, 26.79, 26.75, 26.65, 26.61, 26.03, 25.90, 25.79, 25.68, 22.28, 22.22 ppm; HRMS (ESI) calculated for $C_{49}H_{51}N_2O_{14}S_4^{3-}$ (M) 1019.22, observed 1022.23(M+H), 339.74$(M)^{-3}$, 510.11$(M+H)^{-2}$.

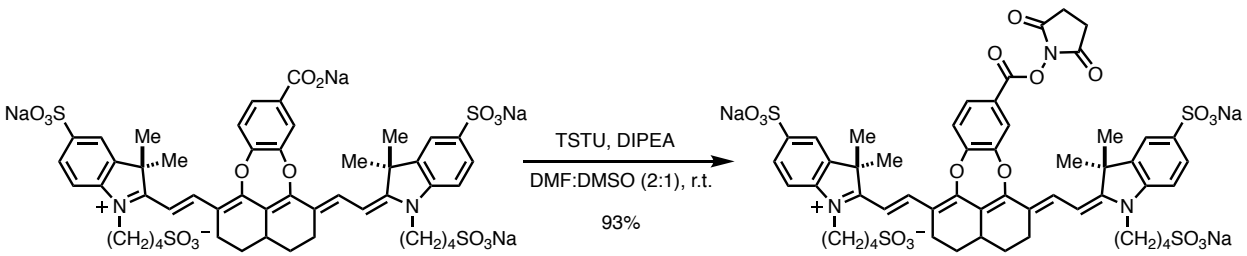


(S4): *β*-alanine *t*-butyl ester hydrochloride (3.0 g, 5.5 mmol) was suspended in saturated aqueous sodium bicarbonate (90 mL) in a round-bottom flask and stirred for 15 minutes at ambient temperature. The reaction mixture was extracted with EtOAc (3 x 50 mL), the combined organic layers dried over $MgSO_4$ and evaporated to give the corresponding free amine (1.8 g) as a redish liquid which was used without further purification. 1,3-propanesultone (1.3 mL, 15 mmol, 1.2 equiv.) and dry THF (25 mL) were charged to the flask and the reaction mixture was refluxed for 2 h during which time a white precipitate formed. The reaction mixture was allowed to cool, filtered and washed with cold acetone and dried under vacuum to afford **S4** in (1.8 g, 54% yield) as a fine white powder. ^{1}H NMR (400 MHz, CD_3OD) δ 3.24 (two overlapping t, J = 7.0 Hz, 4H), 2.93 (t, J = 6.8 Hz, 2H), 2.70 (t, J = 6.8 Hz, 2H), 2.15 (p, J = 7.1 Hz, 2H), 1.48 (s, 9H) ppm; ^{13}C NMR (100 MHz, CD_3OD) δ 171.17, 83.12, 47.95, 44.33, 32.35, 28.28, 22.88, 9.22 ppm; HRMS (ESI) calculated for $C_{10}H_{21}NO_5S$ 268.1213, observed 268.1215.



(FNIR-872): To a microwave vial equipped with a magnetic stir bar was added Compound **FNIR-866** (110 mg, 0.098 mmol, 1 eq), **S4** (78 mg, 0.29 mmol, 3 eq), and HATU (110 mg, 0.29 mmol,

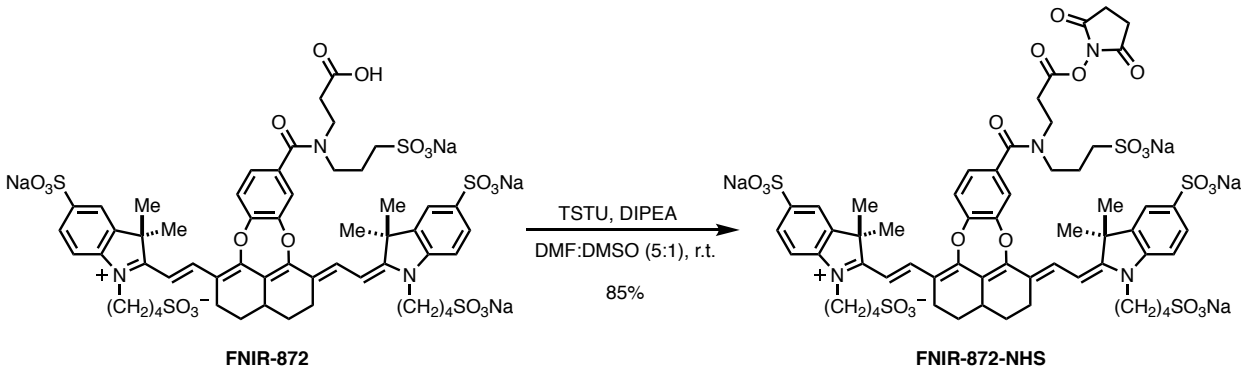
2.0 eq). The vessel was sealed and flushed with argon. DMF (1.5 mL) and DIPEA (86 µL, 0.49 mmol, 5.0 eq) was added and the reaction was heated to 65 °C for 30 min. The reaction mixture was cooled and added to ether (12 mL) in a Falcon tube. The suspension was centrifuged for 5 min at 4500 RPM and the pellet treated with 2 mL phosphoric acid (85 weight % in water) and stirred for 24 h at room temperature. The reaction was diluted with saturated aqueous $NaHCO_3$ (5 mL) and directly purified by reversed-phase chromatography (50 g C_{18} Aq., 0→40% acetonitrile/water). The product-containing fractions were lyophilized to afford **FNIR-872** (59 mg, 45% yield) as a green solid. ^{1}H NMR (400 MHz, CD_3OD) δ 8.68 – 8.62 (dd, 2H), 7.96 – 7.89 (m, 4H), 7.40 – 7.34 (q, 5H), 6.34 – 6.27 (dd, 2H), 4.24 – 4.18 (m, 4H), 3.81 – 3. 67 (d, 4H), 2.99 – 2.92 (m, 8H), 2.68 – 2.64 (m, 6H), 2.15 – 2.13 (d, 3H), 2.03 – 1.98 (m, 10H), 1.90 – 1.85 (m, 12H) ppm; ^{13}C NMR (125 MHz, CD_3OD) δ 172.77, 169.00, 167.93, 146.51, 145.67, 144.09, 143.64, 143.49, 142.57, 141.89, 141.22, 140.90, 140.79, 139.96, 138.73, 136.43, 132.70, 131.47, 129.45, 126.92, 126.78, 123.39, 121.86, 120.01, 119.95, 111.00, 109.70, 104.90, 102.26, 50.44, 50.31, 49.51, 44.27, 43.59, 33.33, 29.61, 29.47, 26.80, 26.76, 26.65, 26.61, 26.04, 25.90, 25.80, 25.68, 22.28, 22.22 ppm; HRMS (ESI) calculated for $C_{55}H_{61}N_3O_{20}S_5^{4-}$ (M) 1243.25, observed 1247.27 (M+4H), 310.81 $(M)^{-4}$, 414.75 $(M)^{-3}$, 622.63$(M+H)^{-2}$.



FNIR-866 **FNIR-866-NHS**

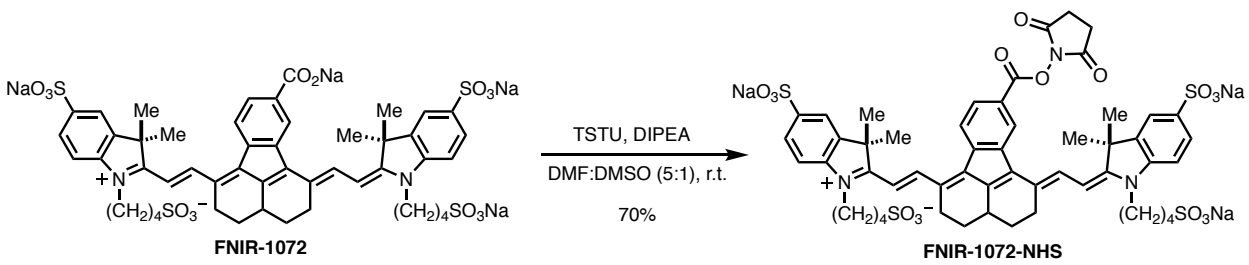
(FNIR-866-NHS): To a microcentrifuge tube containing **FNIR-866** (4.0 mg, 0.0035 mmol, 1.0 eq) was added TSTU (3.2 mg, 0.01 mmol, 3.0 eq), DIPEA (2 µL, 0.01 mmol, 3 eq) and 2:1

DMF:DMSO (300 µL) and the reaction mixture was stirred at room temperature under argon. LCMS analysis indicated complete conversion to the activated NHS ester product in 30 min. The reaction was added to diethyl ether (10 mL) in a 20 mL Falcon tube, resulting in a green precipitate. After centrifugation the pellet was placed under vacuum (<0.1 Torr) for 2 hours, yielding **FNIR-866-NHS** (4.0 mg, 93% yield) as a green solid that was used without further purification. HRMS (ESI) calculated for $C_{53}H_{54}N_3O_{18}S_4^{3-}$ $(M)^{3-}$ 382.7434, observed 382.7443.



FNIR-872 **FNIR-872-NHS**

(FNIR-872-NHS): To a microcentrifuge tube containing **FNIR-872** (13 mg, 0.009 mmol, 1.0 eq) was added TSTU (8.8 mg, 0.029 mmol, 3.0 eq), DIPEA (8.5 µL, 0.048 mmol, 5.0 eq) and 5:1 DMF:DMSO (500 µL) and the reaction mixture was stirred at room temperature under argon. LCMS analysis indicated complete conversion to the activated NHS ester product in 1h. The reaction was inversely added to diethyl ether (10 mL) resulting in a green precipitate. After centrifugation the pellet was placed under vacuum (<0.1 Torr) for 2 hours, yielding **FNIR-872-NHS** (12.0 mg, 85% yield) as green solid that was used without further purification. HRMS (ESI) calculated for $C_{59}H_{64}N_4O_{22}S_5^{4-}$ $(M)^{4-}$ 335.0659, observed 335.0665.



(FNIR-1072-NHS): To a microcentrifuge tube containing **FNIR-1072** (6.5 mg, 0.0060 mmol) was added TSTU (5.4 mg, 0.018 mmol, 3.0 eq), DIPEA (5.2 µL, 0.029 mmol, 5.0 eq) and 5:1 DMF:DMSO (300 µL) and the reaction mixture was stirred at room temperature under argon. LCMS analysis indicated complete conversion to the activated NHS ester product in 3h. The reaction was added to diethyl ether (10 mL) in Falcon tube, resulting in a green precipitate. After centrifugation the pellet was placed under vacuum (<0.1 Torr) for 2 hours, yielding **FNIR-1072-NHS** (5.0 mg, 70% yield) as a redish solid that was used without further purification. HRMS (ESI) calculated for $C_{53}H_{54}N_3O_{16}S_4^{3-}$ $(M)^{3-}$ 372.0801, observed 372.0811.

FNIR-Tag-Dextran (10 kDa): Amino-Dextran-10 kDa (500 µg) was dissolved in 225 µL of 100 mM PBS (pH 8.4) in a microcentrifuge tube. FNIR-Tag-NHS (4 eq, 20 µL of a 10 mM DMSO stock solution) and 5 µL of DMSO were added to give a final DMSO content of 10%. The microcentrifuge tube was shielded from light and gently rocked on an orbital shaker at 500 RPM for 1 h. The conjugate solution was filtered through a water-equilibrated centrifugal filter (Amicon Ultra-0.5 mL, 3kDa MWCO, Millipore Sigma) according to the package instructions. The concentrated conjugate solution was resuspended in water (400 µL) and centrifuged repeatedly until the filtrate showed no detectable free dye (5 times total), as determined by Nanodrop. The conjugate solution was lyophilized to afford FNIR-Tag-Dex (10 kDa) (690 µg) as a fluffy green powder.

FNIR-872-Dextran (70 kDa): Amino-Dextran-70 kDa (400 μg) was dissolved in 180 μL of 50 mM PBS (pH 7.4) in a microcentrifuge tube. FNIR-872-NHS (4 eq, 2.4 μL of a 10 mM DMSO stock solution) and 17.6 μL of DMSO were added to give a final DMSO content of 10%. The microcentrifuge tube was shielded from light and gently rocked on an orbital shaker at 500 RPM for 1 h. The conjugate solution was filtered through a water-equilibrated Zeba spin desalting column (7 kDa MWCO, Thermo Fisher Scientific) and the filtrate was dialyzed against water using a Thermo Fisher Scientific mini-dialysis device (3 kDa MWCO) for 3h, followed by another 16 h after buffer exchange. The conjugate solution was lyophilized to afford FNIR-872-Dex (70 kDa) (0.5 mg) as a fluffy brown powder.

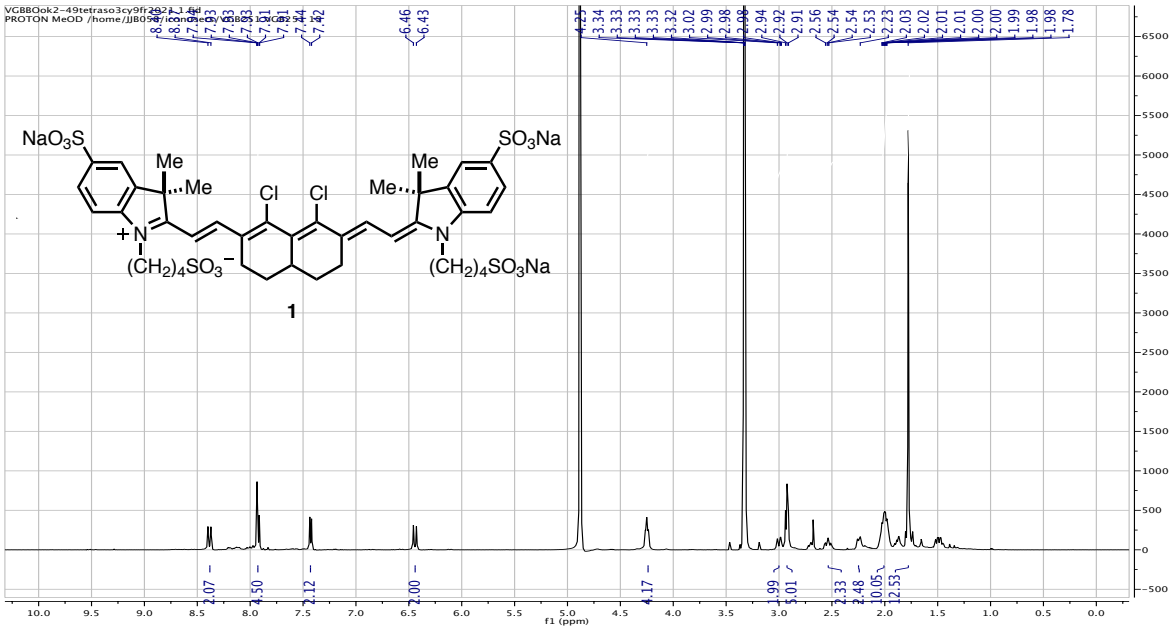
FNIR-1072-Dextran (10 kDa): Amino-Dextran-10 kDa (1.0 mg) was dissolved in 112.5 μL $Na_2B_4O_7$ buffer (0.1 M. pH 8.5) in a microcentrifuge tube. FNIR-1072-NHS (4 eq, 4 μL of a 100 mM DMSO stock solution) and DMSO (8.5 μL) were added to give a final DMSO content of 10%. The microcentrifuge tube was shielded from light and gently rocked on an orbital shaker at 500 RPM for 16 h. The conjugate solution was filtered through a water equilibrated Zeba spin desalting column (7 kDa MWCO, Thermo Fisher Scientific) and the filtrate was dialyzed using a Thermo Fisher Scientific mini-dialysis device (3 kDa MWCO) against water for 3h, followed by another 16 h after buffer exchange. The conjugate solution was lyophilized to afford FNIR-1072-Dex (10 kDa) (1.8 mg) as a brown fluffy solid.

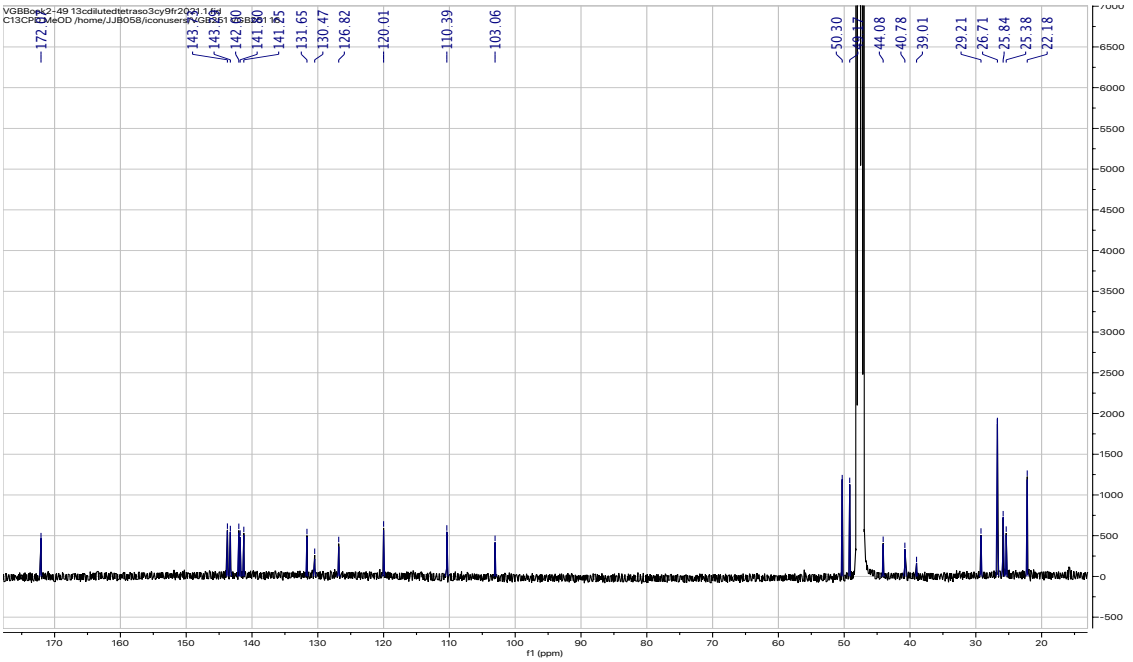
Spectral Characterization of Fluorophore Dextran Conjugates

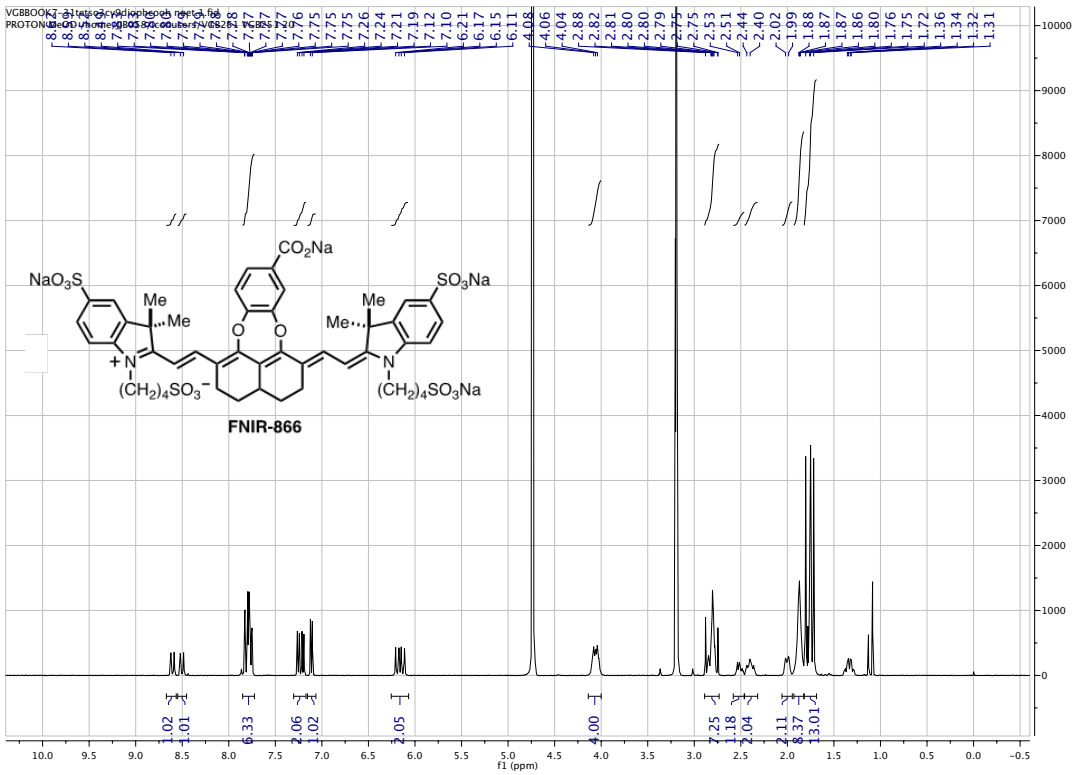
After purification of the fluorophore-dextran conjugates, the aqueous solution was lyophilized, and the resulting solid material was resuspended in water at a concentration of 1 mg/mL. The

effective dye concentration of the sample was determined on a diluted sample in PBS using Beer's law (ε = 200,000 $M^{-1}cm^{-1}$ for FNIR-Tag, ε = 145,000 M^{-1} cm^{-1} for FNIR-872 and ε = 70,000 M^{-1} cm^{-1} for FNIR-1072). The solution was filtered through a 0.22 μM sterile filter (Acrodisc), aliquoted into doses with 75 nmol effective dye amount, lyophilized and the aliquots were stored at –80 °C.

^{1}H and ^{13}C NMR Spectra



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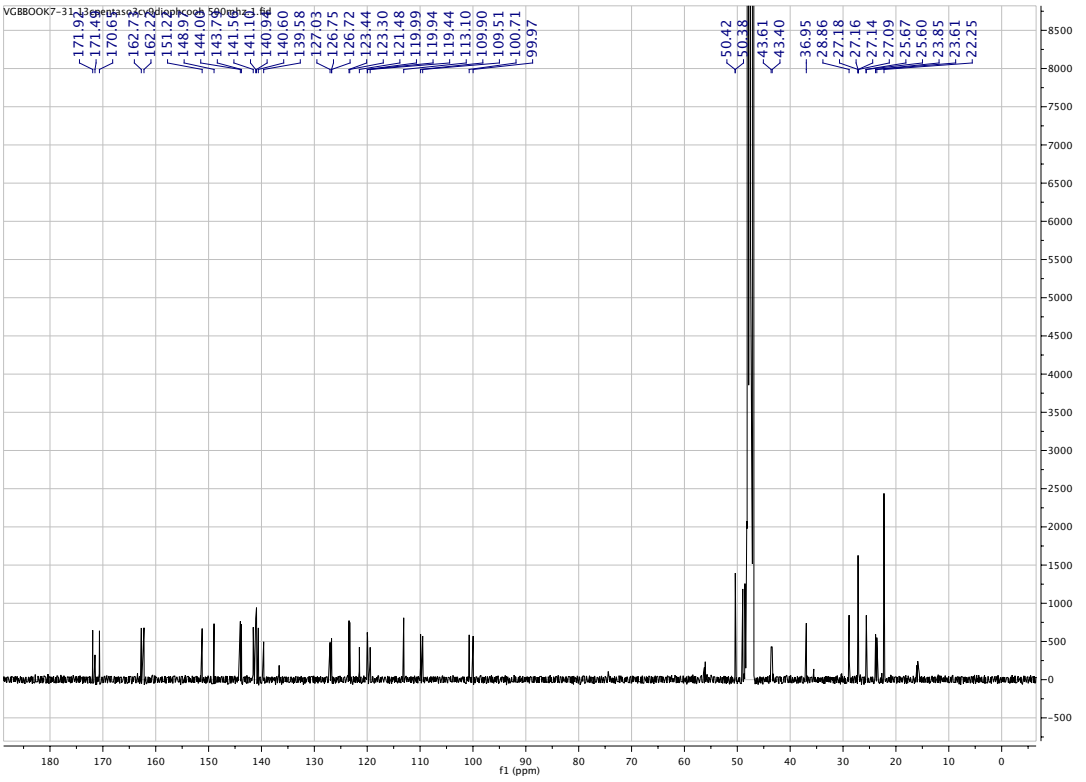
NaO3S
SO3Na
Me
Me
Me
Me
O
O
+N
(CH2)4SO3−
N
(CH2)4SO3Na
FNIR-866
f1 (ppm)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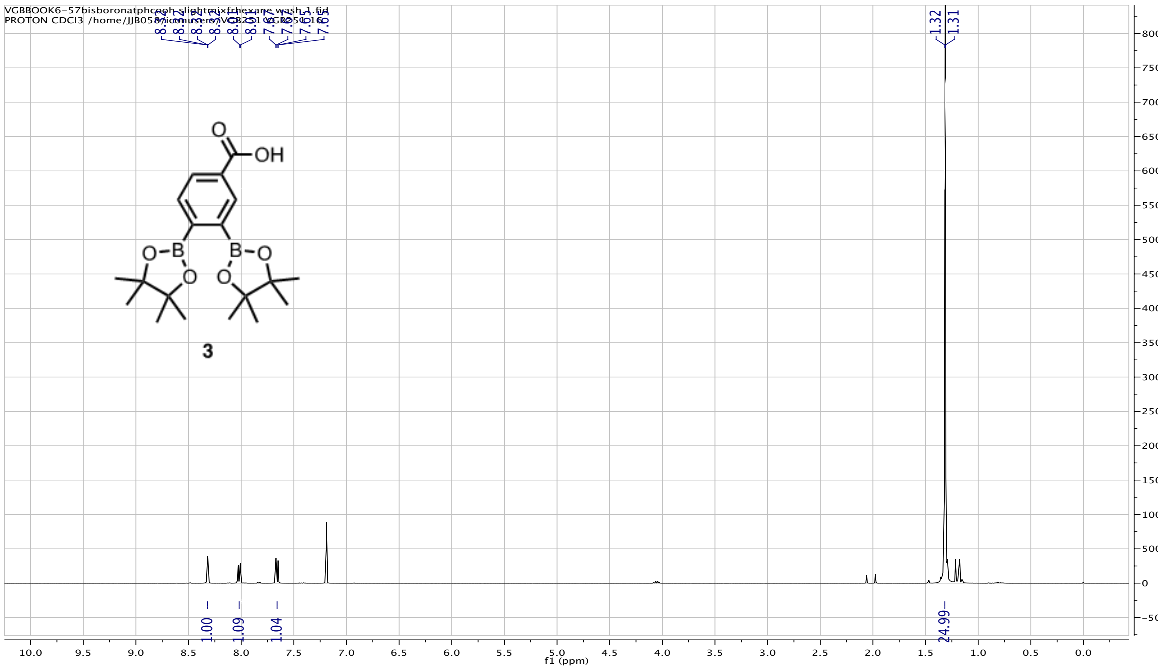
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1.00
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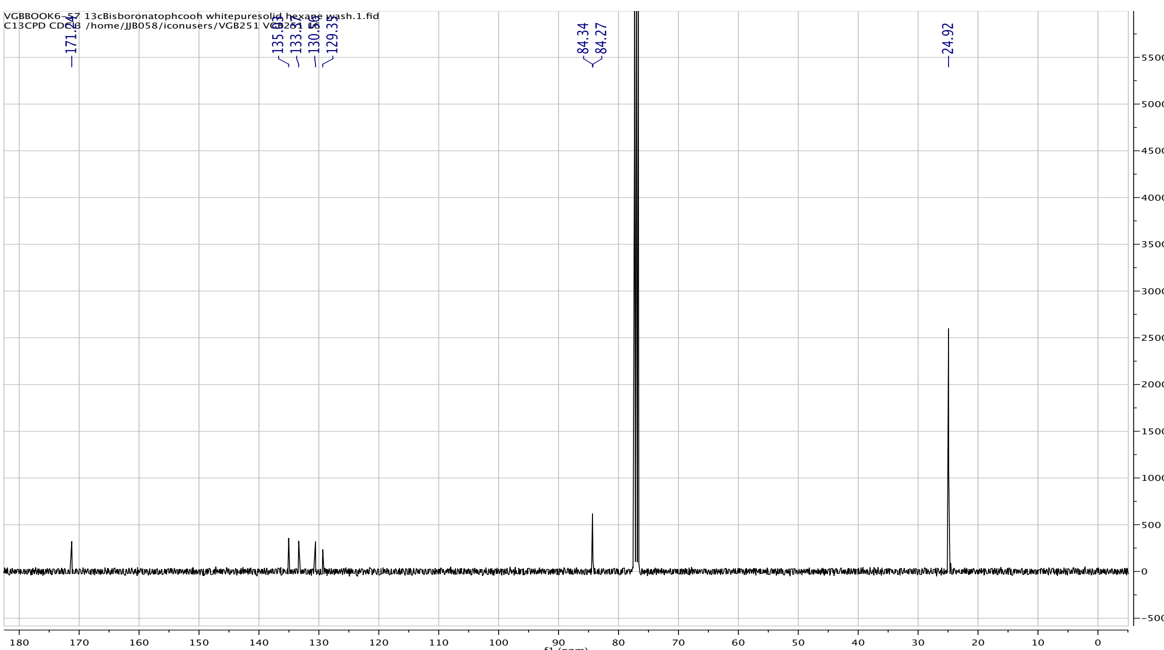
24.99
f1 (ppm)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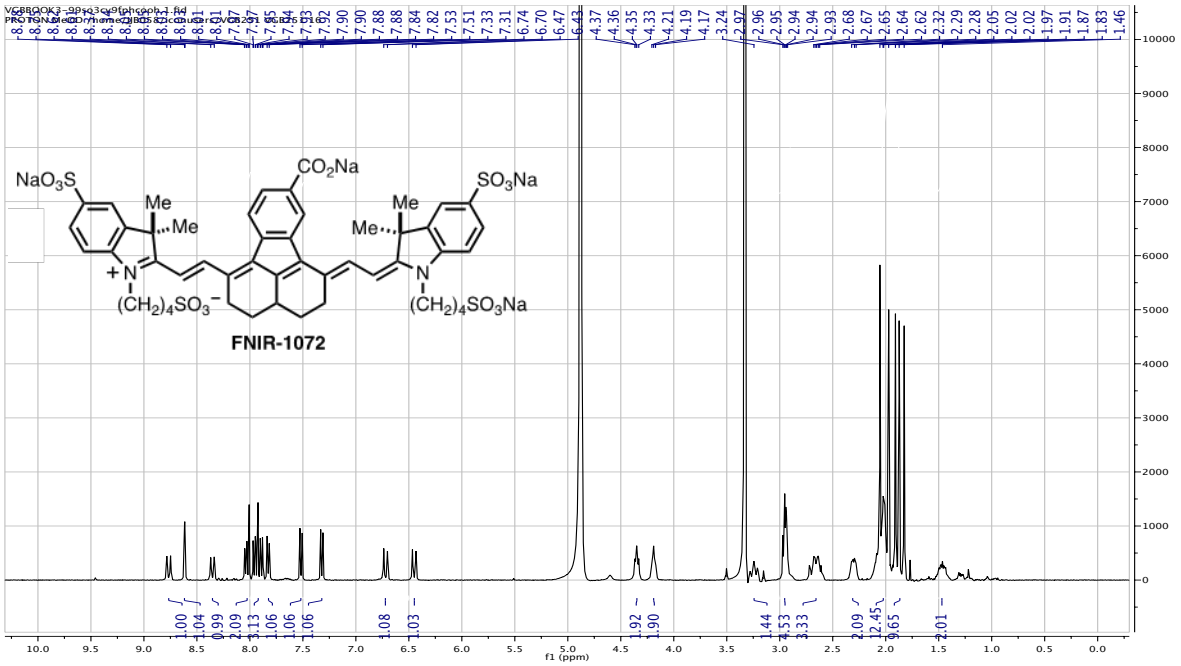
24.92
f1 (ppm)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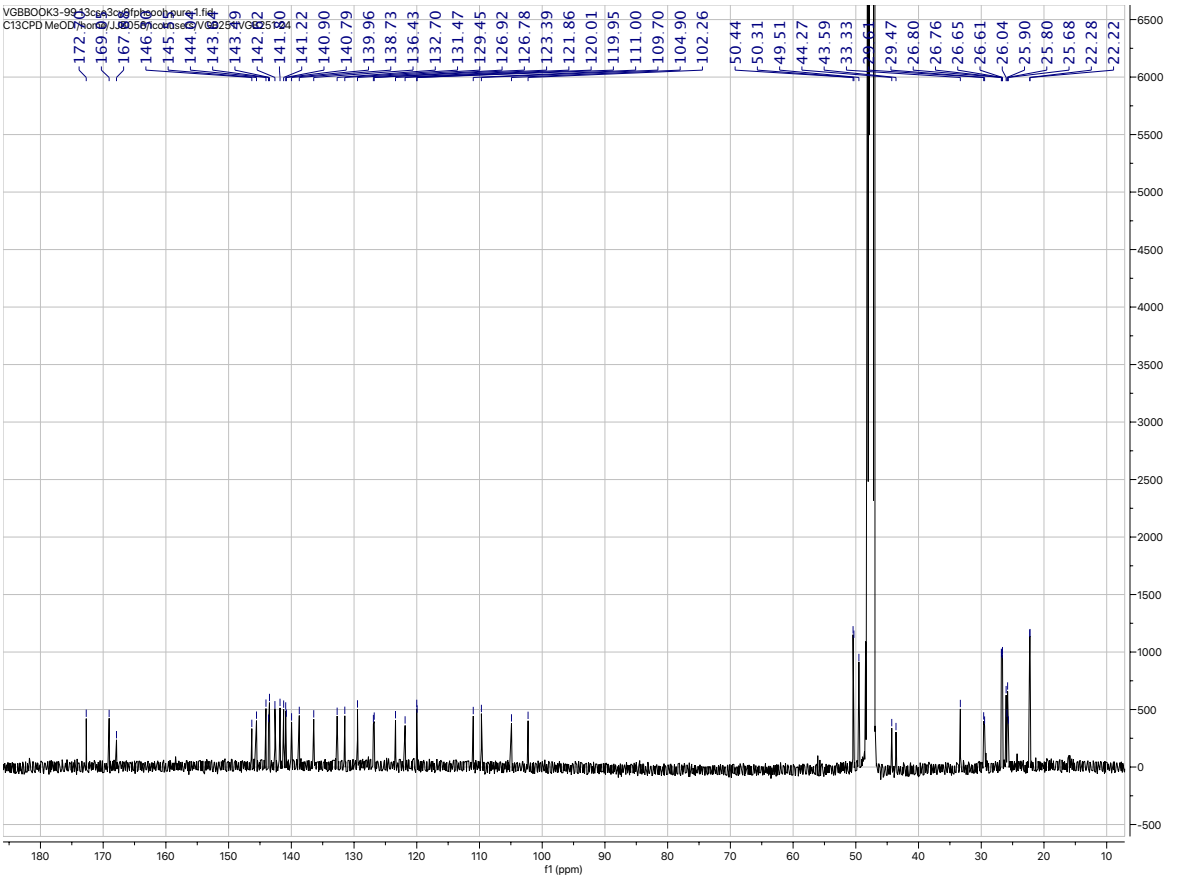
FNIR-1072
f1 (ppm)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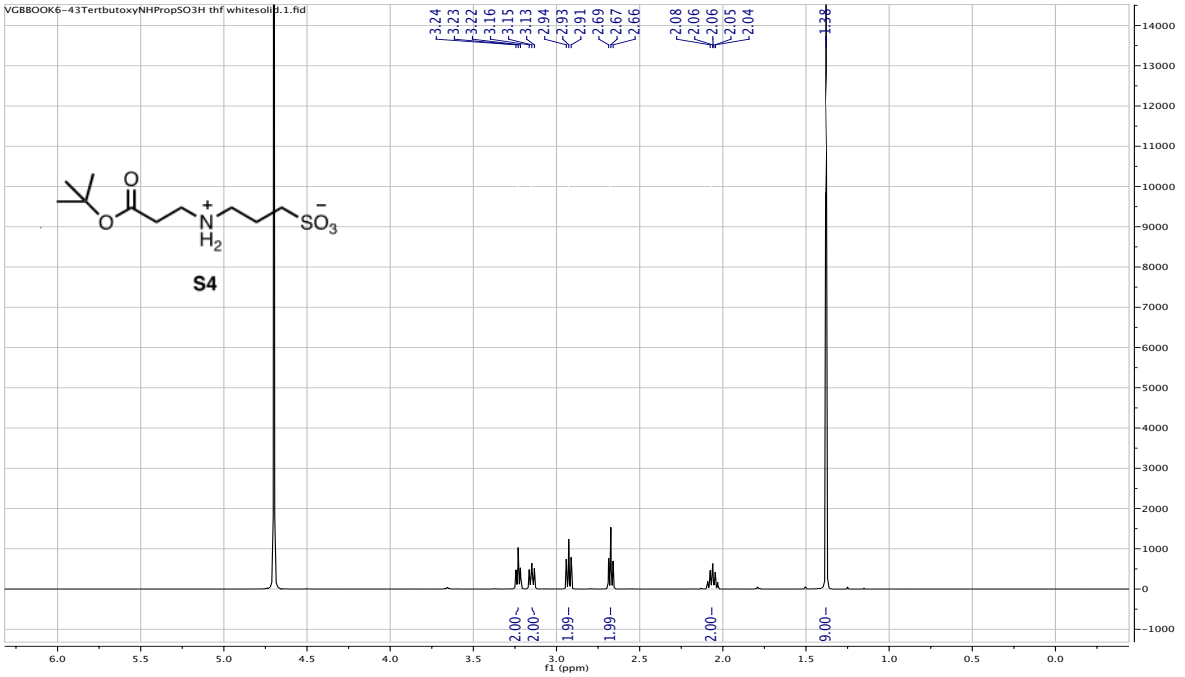
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2.91
2.69
2.67
2.66
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2.06
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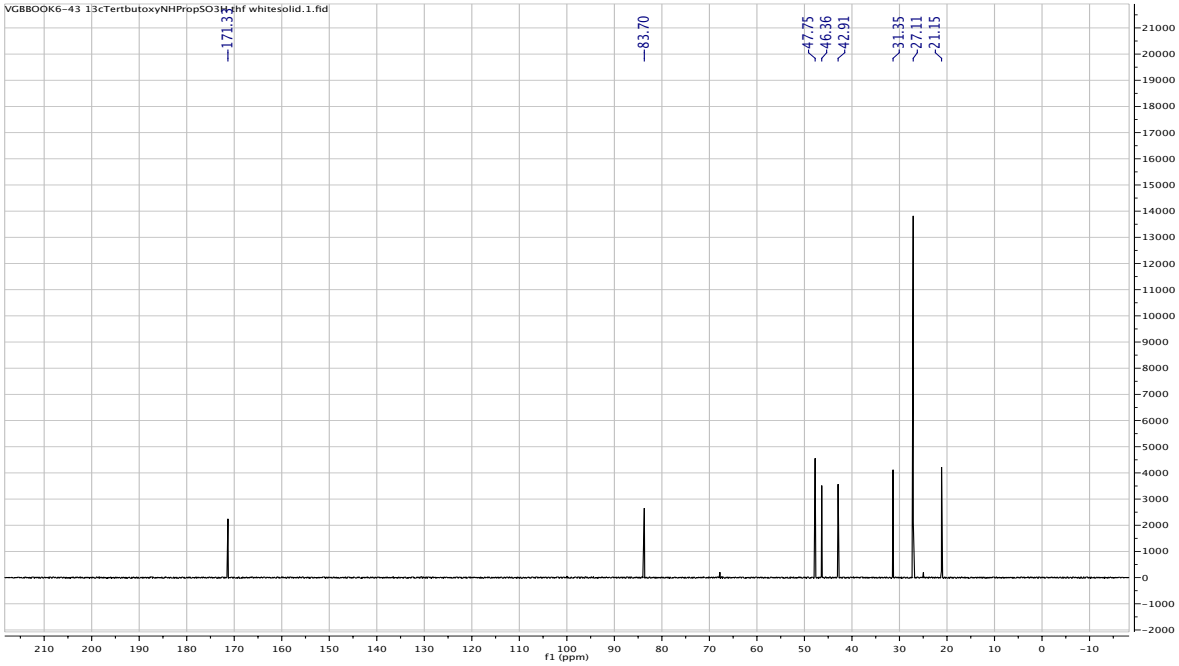
9.00
f1 (ppm)

S4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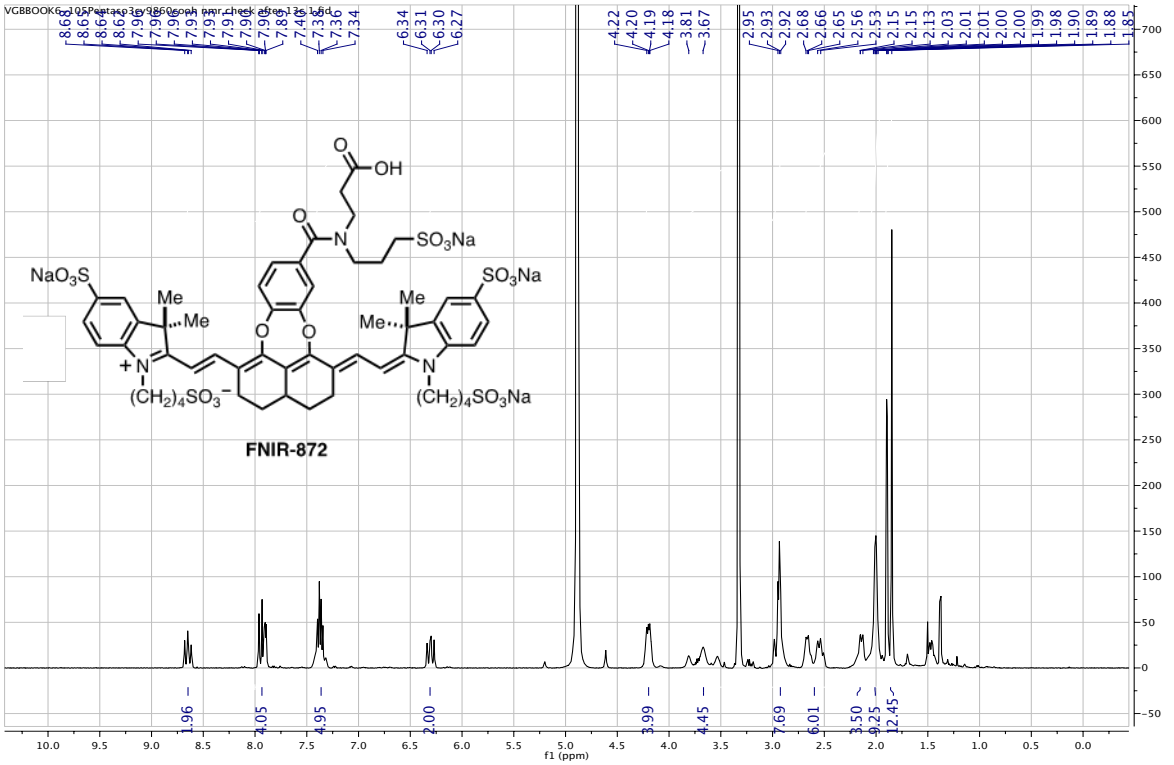
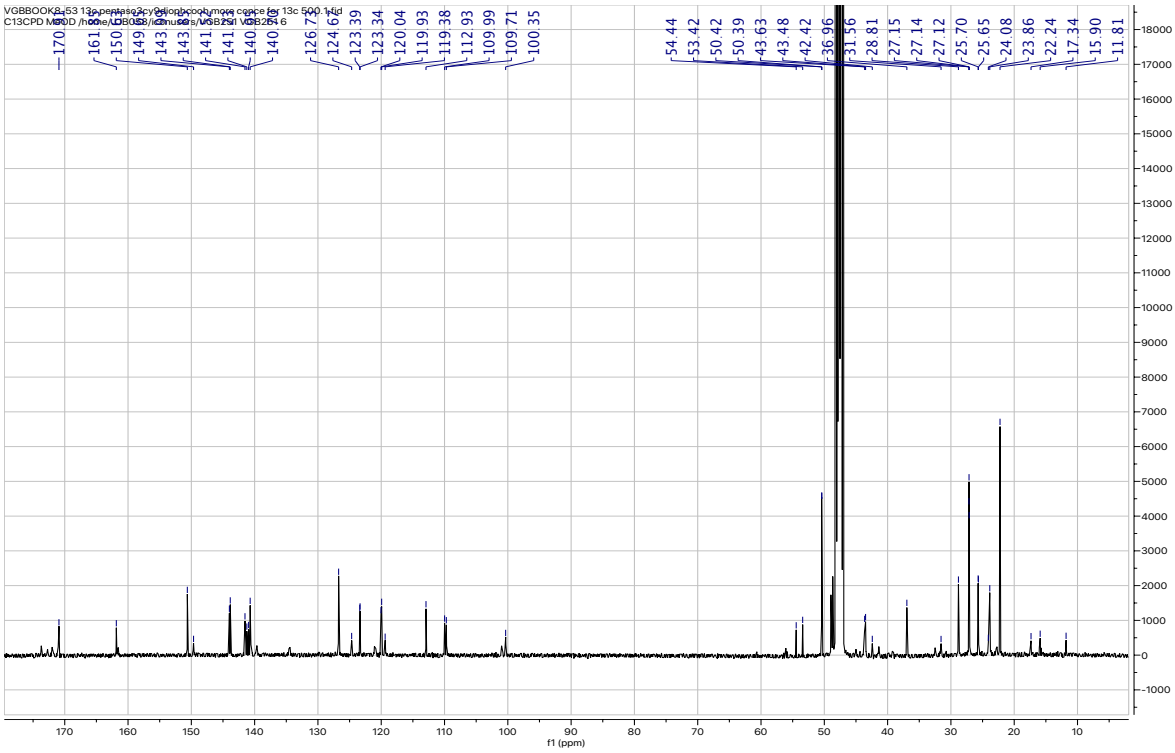
f1 (ppm)


FNIR-872



Supplementary Note 3: SWIR Imaging Setup

The home-built shortwave infrared (SWIR) setup utilizes LuOcean Mini 785 nm (LU0785DLU250-S70AN03, 25 W), 890 nm (LU0890D400-U10AF, 40W) and 1064 nm (LU0980D350-D30AN, 35W) diode lasers (Lumics, Berlin, Germany) as the excitation sources coupled through a multimode fiber cable (Thorlabs, BF46LS01) and directed to a 1" broadband dielectric elliptical mirror (750-1100 nm) (Thorlabs, BBE1-E03) housed in a kinematic mirror mount (Thorlabs, KCB1E). The aligned beams are then passed through an achromatic doublet (Thorlabs, AC254-050-AB-ML), square engineered diffuser (Thorlabs, ED1-S20-MD) and 1" short pass filters (i.e. Edmund Optics, 64-339) for cutting out excess light from laser excitation. The laser power as measured at the surface of the subject was ~80-100 mW/cm^2 for the 785 and 890 nm laser lines.

Filtering and detection of SWIR emission was enabled by various 50 mm-diameter long pass filters (e.g. Edmund optics, 89-665) placed in lens tubing and directed to either a NIRvana 640ST (Princeton Instruments) or Goldeye G-032 (Allied Vision) SWIR camera fitted with a SWIR compatible lens (f = 35 mm, Navitar SWIR-35). IR-light brightfield images were recorded using a heat lamp or 1300 nm LED excitation. For whole body imaging of the orthotopically implanted breast MDA-MB-468 tumors as well as for multi-color video-rate imaging experiments, the custom-built setup presented the same laser fiber-optic bundle and cage system described above as excitation source, in combination with 2X 1" 1100nm short pass filters (Edmund Optics 64-339). Specific emitted fluorescence from the stage was directed through a custom filter set defined for each experiment: 1) 2X 2'' 1000nm long pass filters or 2) 1X 2'' 1100nm long pass filter in combination with 1X 2'' 1150nm long pass filter and 2X 1'' 1150nm filters and ultimately

acquired by Allied Vision Goldeye G-032 Cool TEC2 camera equipped with the Navitar, SWIR-35 lens and located right above the stage.

The scheme for synthesizing the laser pulses and acquisition was described previously.[28]

A GUI application (Camera Control and Data Acquisition, CCDA) https://gitlab.com/brunslab/ccda was developed in MATLAB for acquisition, visualization, microcontroller unit (MCU) control and experiment documentation. It allows programming the MCU with an externally edited Arduino sketch, setting a sequence of trigger pulses to the camera and the illumination devices (IDs) to be looped by the MCU. The contents of the sketch are saved together with all other settings in a metadata file. The trigger loop is started with a button sending a serial signal to the MCU. Custom data acquisition is used to allow taking videos of indefinite length by writing data directly to disk at full color depth.[29] Three modes of acquisition are enabled through CCDA:

1. Continuous mode – where the camera acquires as fast as possible at a predefined exposure time and illumination is externally and asynchronously turned on and off.
2. Rising Edge Camera Trigger – the camera exposes for a predefined time after receiving the rising edge of a trigger pulse. Effective exposure between channels is varied by controlling the length of the ID on-time through its trigger pulse length. All channels have the dark noise of the longest exposure channel, and framerate is limited to $\frac{1s}{channels \times longest\ exposure}$

[28] Cosco, E. D.; Spearman, A. L.; Ramakrishnan, S.; Lingg, J. G. P.; Saccomano, M.; Pengshung, M.; Arus, B. A.; Wong, K. C. Y.; Glasl, S.; Ntziachristos, V.; Warmer, M.; McLaughlin, R. R.; Bruns, O. T.; Sletten, E. M., Shortwave infrared polymethine fluorophores matched to excitation lasers enable non-invasive, multicolour in vivo imaging in real time. *Nat. Chem.* **2020**.

[29] Rolf Harkes (2021). Multi-image Tiff Writer (https://github.com/rharkes/Fast_Tiff_Write), GitHub. Retrieved May 30, 2021

3. Level High Camera Trigger – the camera exposes only for the duration of the trigger pulse, which is synchronized with the one to the ID. This cannot circumvent the framerate limitations (100 fps for the Goldeye G-032 camera) coming from the camera readout time but optimizes it when channels have different exposure times and reduces dark noise in the lower effective exposure channels.

Additionally, CCDA enables the user to conduct "live multicolor imaging" by deinterleaving the acquired image sequence and showing a separated live preview of each channel while acquiring in real-time. Each channel preview window has individual brightness adjustment sliders to adjust the corresponding fluorescent intensity and avoid saturation or to better display lower signals. One of these channels is commonly reserved for an LED emitting above the employed emission filter in the set-up thus obtaining a so-called reflection channel. In an intra-operative context, the reflection channel gives not only accurate anatomical visualization of the mouse (room-light-like view) but also helping to localize the fluorophores excited in the other channels.

Lastly, channels can be automatically merged into a single multiplexed RGB live video while each channel can be selected as one of the RGB color bands of the multiplexed preview. The brightness adjustments from the individual channel previews are carried over into the multiplexed image as well. This offers a clear overview of the intensity of the different fluorophores simultaneously throughout the image.

The CCDA can be found at https://gitlab.com/brunslab/ccda and the version used throughout the work in this paper is release v3.0.1beta. Currently only Allied Vision GoldEye GigE cameras are supported.

Supplementary Note 4: Figure 2 and 3 Acquisition Settings

Fig 2c. Images were acquired on a NIRvana 640ST using 3x 1150 long pass filters. The lasers (785 nm for IR-800CW-Pan, 890 nm for FNIR-872-Pan and 1064 nm for FNIR-1072-Pan) were power matched at 100 mW/cm2 measured over the tumor. Camera exposure times were 150-250 ms, 250-400 ms and 400-800 ms for the IR-800CW, FNIR-872 and FNIR-1072 channels, respectively.

Fig 3b. Images were acquired on a NIRvana 640ST using three 1150 long pass filters. The lasers (785 nm for ICG and 890 nm for FNIR-872-Dex) were power matched at 100 mW/cm^2 measured over the tumor for each imaging timepoint. Camera exposure times were 400 ms and 300 ms for the ICG and FNIR-872-Dex channels, respectively

Fig 3-g. Images were acquired on a Allied Vision Goldeye G-032 Cool TEC2 camera equipped with the Navitar, SWIR-35 lens. (Ch. 1: Reflection/1300 nm LED 10 ms; Ch. 2: ICG/785 nm Laser 80 mW/cm^2 10 ms; Ch. 3: FNIR-872-Pan/892 nm Laser 115mW/cm^2 10-50ms; Ch4: FNIR-1072-Dex/968 nm Laser 660 mW/cm^2 25-50 ms – Camera exposure time 50 ms)