Supplementary Information

for

Excited state iminium form can explain the unexpected solvatochromic behavior of symmetric 1,5-and 1,8-diaminonaphthalenes.

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Experimental

Materials and Methods

1,5-DAN: 1,5-diamino naphthalene:

CAS: 2243-62-1

MW: 158.2 g/mol

From: Acros organics, Cat: 112290250

1,8-DAN: 1,8-diamino naphthalene:

CAS: 479-27-6

MW: 158.2 g/mol

From: Sigma-aldrich, Cat: D21405-5G

Acetone, dichloromethane (DCM), hexane, 2-propanol (iPrOH), toluene, ethyl-acetate (EtOAc) (reagent grade, Molar Chemicals, Hungary) were purified by distillation. Acetonitrile (MeCN), tetrahydrofuran (THF), methanol (MeOH), dimethyl formamide (DMF), dimethyl sulfoxide (DMSO), pyridine (HPLC grade, VWR, Germany), cyclohexane, 1,4-dioxane (reagent grade, Reanal, Hungary), were used without further purification. Other solvents and reagents were purchased from Sigma Aldrich in reagent grade and used as received.

UV–vis: The UV–vis spectra were recorded on a UV-6300PC double beam spectrophotometer (VWR International) in a quartz cuvette of 1.00 cm optical length. A 3.00 cm^3 solution was prepared from the sample. Background was recorded for the pure solvent in the reference cuvette.

Steady-state fluorescence measurements were carried out using a Jasco FP-8550 fluorescence spectrophotometer equipped with a Xe lamp light source. The excitation and emission spectra were recorded at 20 °C, using 2.5 nm excitation, 2.5 nm emission bandwidth and 200 nm/min scanning speed. Fluorescence quantum yields (Φ_F) were calculated by using quinine-sulfate as the reference, using the following equation:

$$\Phi_F = \Phi r * \frac{I}{I_{ref}} * \frac{A_{ref}}{A} * \frac{n^2}{n_{ref}^2}$$

where Φ_r is the quantum yield of the reference compound (quinine-sulfate in 0.1 mol/L perchloric acid, absolute quantum efficiency (Φ_r = 55%)), *n* is the refractive index of the solvent, *I* is the integrated fluorescence intensity and *A* is the absorbance at the excitation wavelength. The absorbances at the wavelength of excitation were kept below *A* = 0.1 in order to avoid inner filter effects.

For UV–vis and fluorescence measurements, the investigated compounds were dissolved in acetonitrile at a concentration of 3.11 mM and were diluted to 1.05×10^{-5} M (1,5-DAN) and 1.38×10^{-5} M (1,8-DAN) in the solvents in interest. The spectra were processed using Spectragryph software.

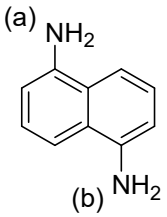
Summary table of the photophysical properties of 1,5-DAN and 1,8-DAN

Table S1. The absorption maximum wavelengths (λ_{Abs}), the molar extinction coefficients at λ_{Abs} (ε) the fluorescence emission maxima (λ_{Em}) the quantum yields (Φ_f) determined in various solvents for 1,5-diaminonaphthalene (**1,5-DAN**) and 1,8-diaminonaphthalene (**1,8-DAN**). The dielectric constants of the solvents (ε_r)* are listed next to the solvent names.

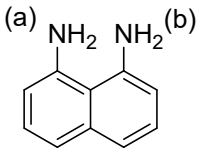
Solvent (ε_r)	1,5-DAN						1,8-DAN					
	λ_{Abs} (nm)	$\varepsilon \times 10^{-3}$ ($M^{-1}cm^{-1}$)	λ_{Ex} (nm)	λ_{Em} (nm)	Φ_f (%)	$\Delta\nu_{SS}$ (cm^{-1})	λ_{Abs} (nm)	$\varepsilon \times 10^{-3}$ ($M^{-1}cm^{-1}$)	λ_{Ex} (nm)	λ_{Em} (nm)	Φ_f (%)	$\Delta\nu_{SS}$ (cm^{-1})
n-Hexane (1.88)	321	9.97	329	367	50.0	3904	347	8.29	347	398	16.5	3693
Dioxane (2.21)	334	13.6	344	377	49.4	3414	351	10.5	351	407	15.2	3920
Toluene (2.37)	331	12.7	342	374	40.8	3474	350	8.98	350	406	21.2	3941
EtOAc (5.99)	332	12.1	333	376	34.0	3525	350	8.93	350	410	16.4	4181
THF (7.58)	336	12.3	344	378	39.8	3307	351	9.55	351	411	15.0	4159
DCM (8.93)	332	11.7	319	374	7.6	3383	349	8.79	335	414	17.5	4499
Pyridine (12.4)	349	13.0	-	-	-	-	354	10.2	-	-	-	-
2-propanol (19.3)	330	11.7	329	392	43.1	4793	334	8.78	336	425	27.5	6411
Acetone (20.5)	344	12.5	343	383	1.6	2960	350	9.19	350	411	2.3	4241
Methanol (32.6)	328	12.1	329	391	39.9	4912	335	8.76	346	426	15.8	6377
DMF (37.2)	348	14.1	349	383	51.5	2626	353	9.91	353	415	23.2	4232
Acetonitrile (35.7)	333	12.4	333	377	37.4	3505	350	8.93	350	416	21.9	4533
DMSO (46.8)	351	15.9	351	387	63.1	2650	354	10.8	355	416	27.3	4210
Water (78.4)	324	10.8	314	406	36.2	6234	329	8.10	329	439	7.5	7616

*The dielectric constants were collected from the Gaussian website and are the same as used by Gaussian 16 software when CPCM solvent model is set during calculations. (https://gaussian.com/scrf/?fbclid=IwAR3IfO9eGH_hadhxrrPJZbiFQoaGsYrmTd_foD8wqP6Ny3vGxZDX3VAa94). They are rounded to three significant digits and only serve as a measure to order the solvents according to increasing solvent polarity.

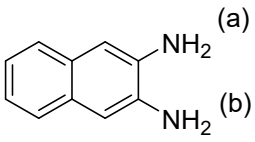
1,5-diaminonaphthalene
1,5-DAN



1,8-diaminonaphthalene
1,8-DAN



2,3-diaminonaphthalene
2,3-DAN



Scheme S1. Chemical structures of 1,5- 1,8- and 2,3-diaminonaphtalenes (1,5-DAN, 1,8-DAN and 2,3-DAN)

Fluorescence properties of 1,5-DAN

Steady state emission spectra

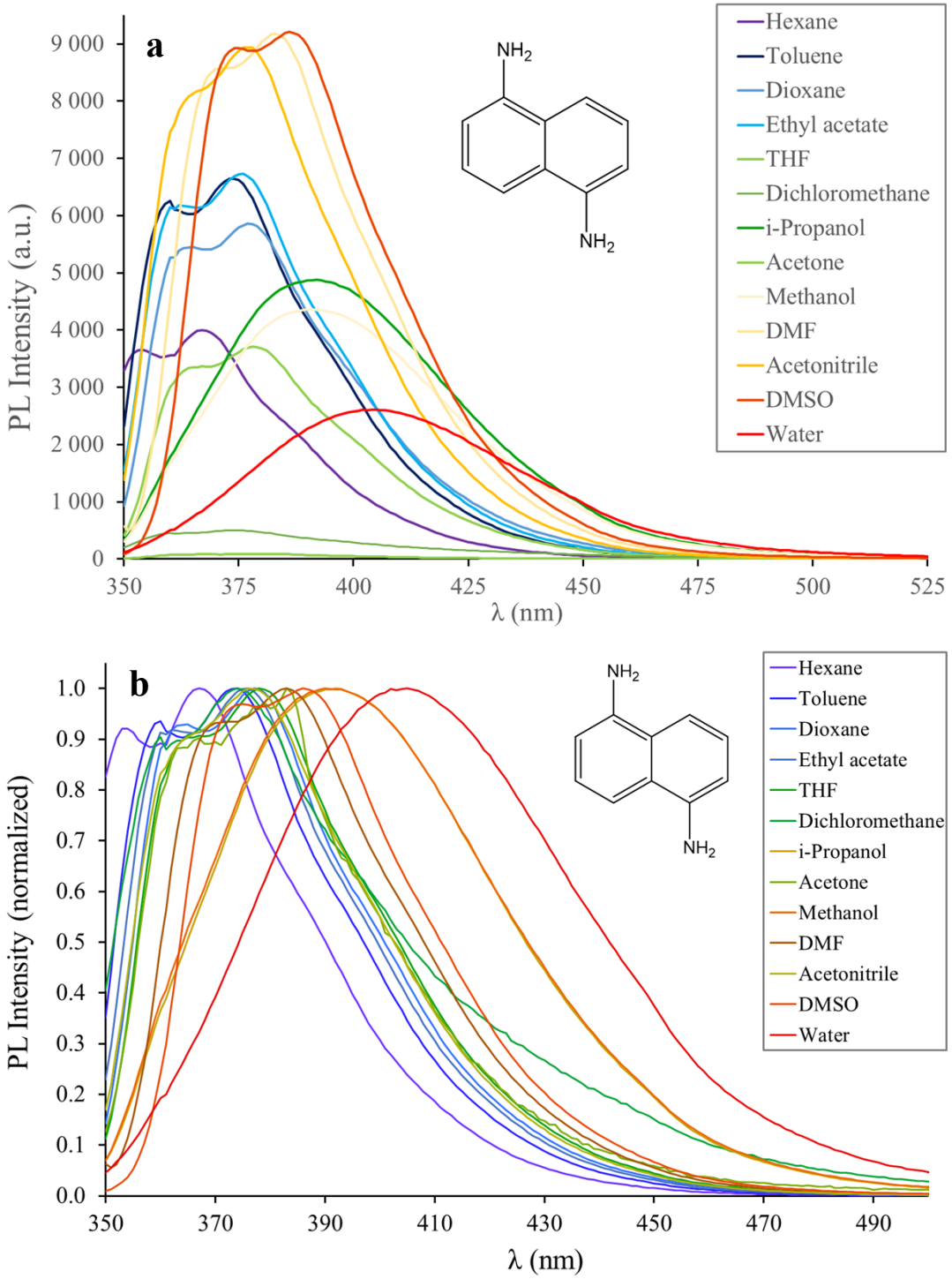


Figure S1. (a) Steady-state fluorescence spectra of 1,5-DAN recorded in various solvents of different polarity. (**b**) The normalized emission spectra. ([dye] = 1.05×10^{-5} M, T=20 ºC).

Excitation spectra of 1,5-DAN

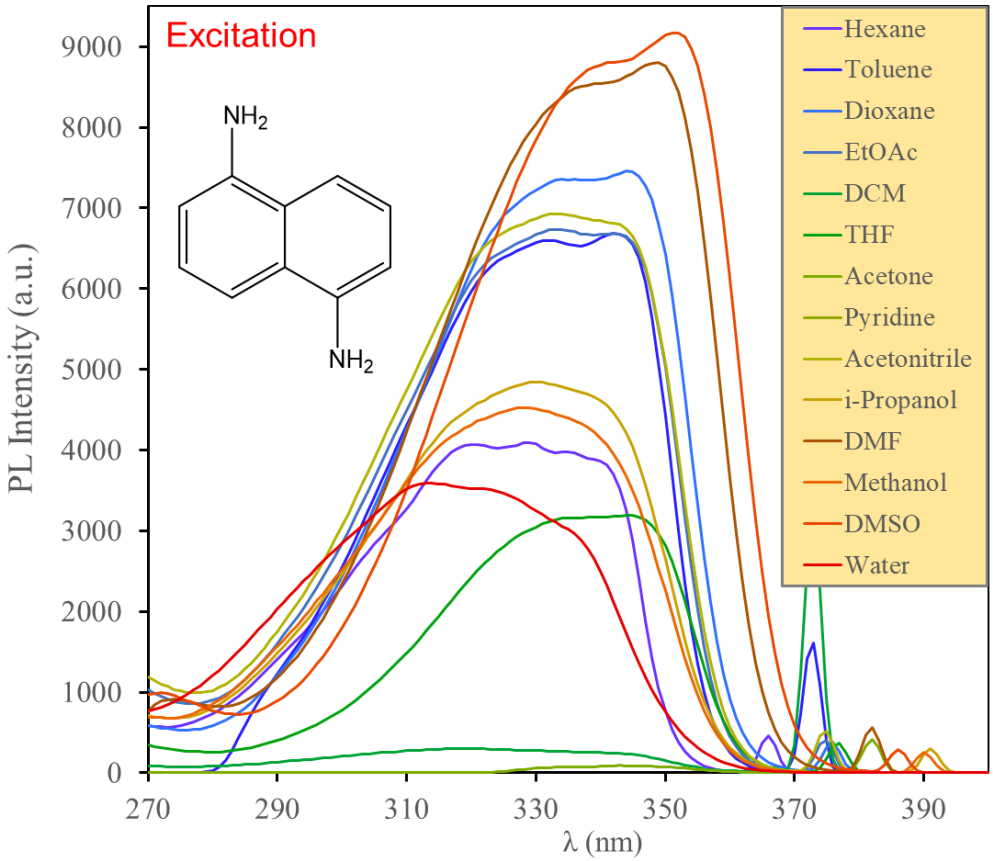


Figure S2. Excitation spectra of 1,5-DAN recorded in various solvents of different polarity. ([dye] = 1.05×10^{-5} M, T=20 ºC).

Emission spectra of 1,5-DAN recorded in alcohols

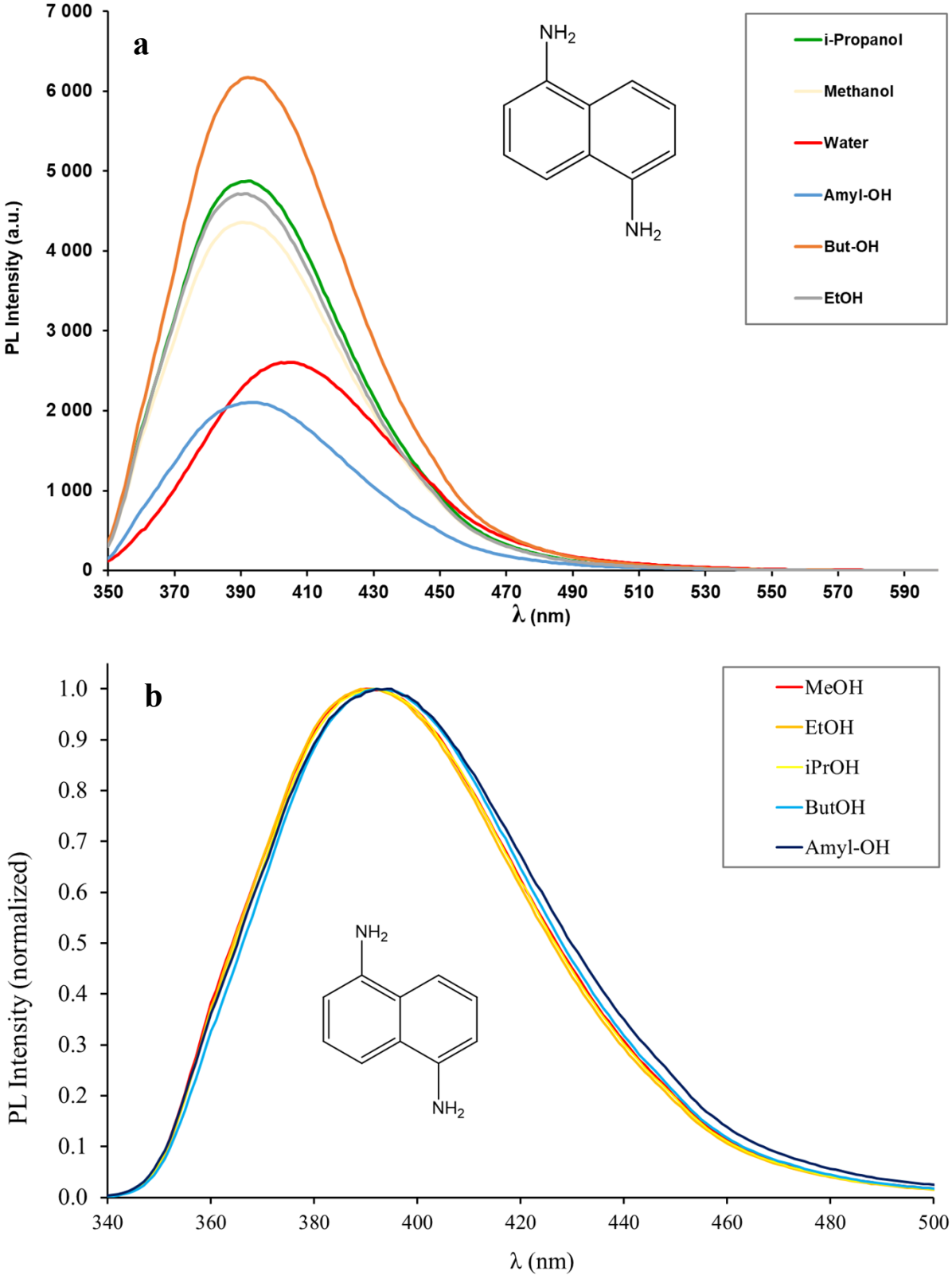


Figure S3. (a) Steady-state fluorescence spectra of 1,5-DAN recorded in various primary alcohols. (**b**) The normalized emission spectra. ([dye] = 1.05×10^{-5} M, T=20 ºC).

Fluorescence properties of 1,8-DAN

Steady state emission spectra

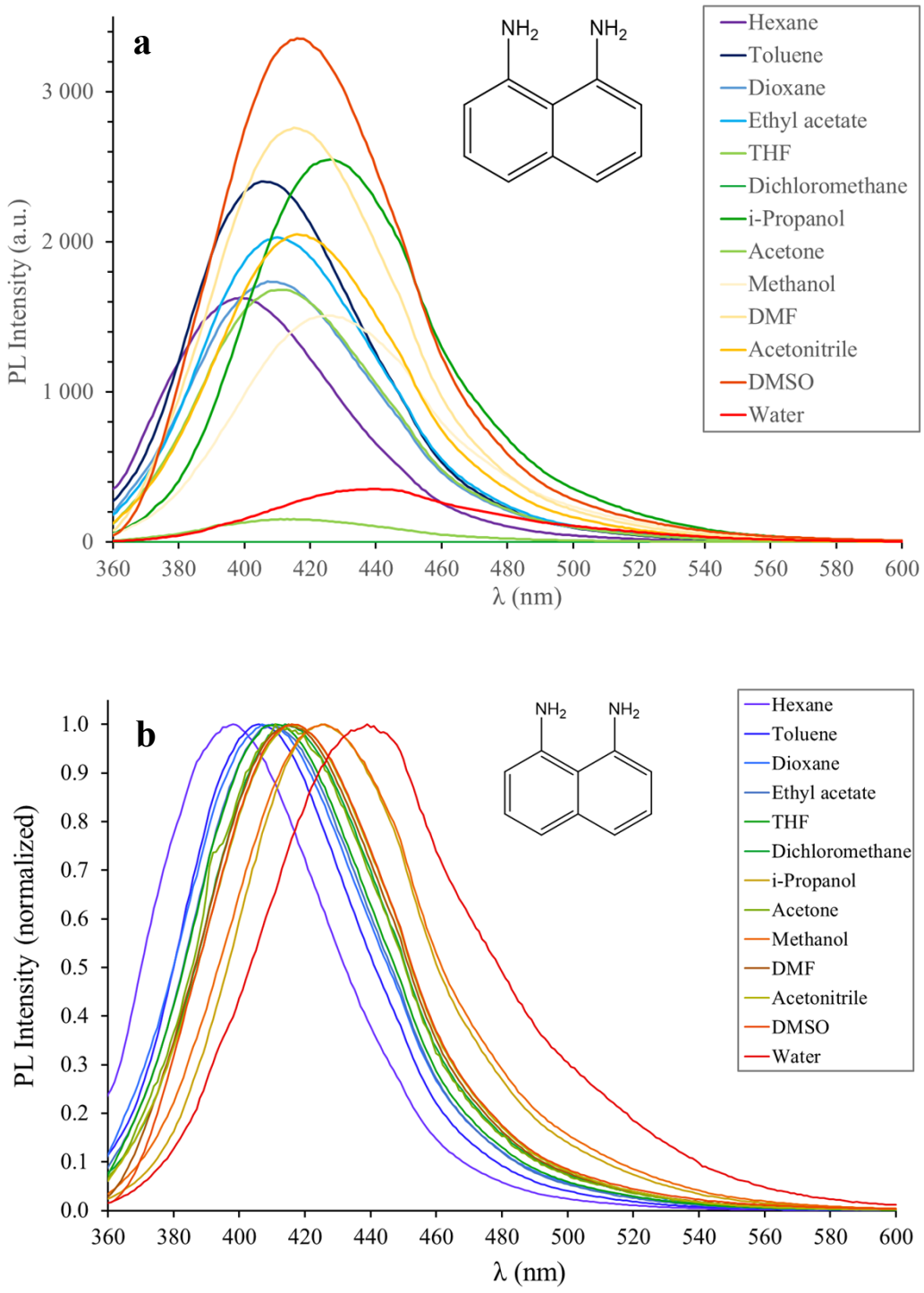


Figure S4. (a) Steady-state fluorescence spectra of 1,8-DAN recorded in various solvents of different polarity. (**b**) The normalized emission spectra. ([dye] = 1.13×10^{-5} M, T=20 ºC).

Excitation spectra of 1,8-DAN

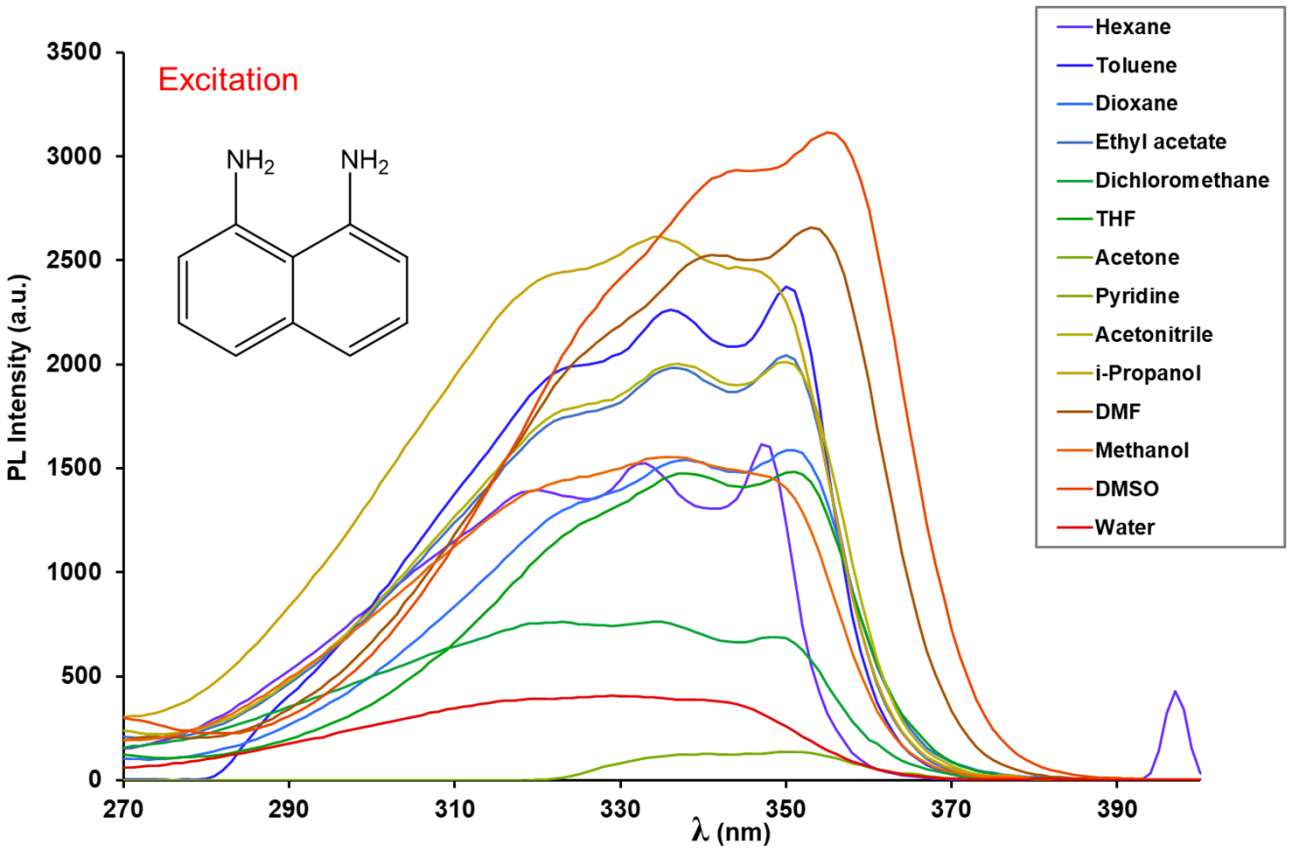


Figure S5. Excitation spectra of 1,5-DAN recorded in various solvents of different polarity. ([dye] = 1.13×10^{-5} M, T=20 ºC).

Emission spectra of 1,8-DAN recorded in alcohols

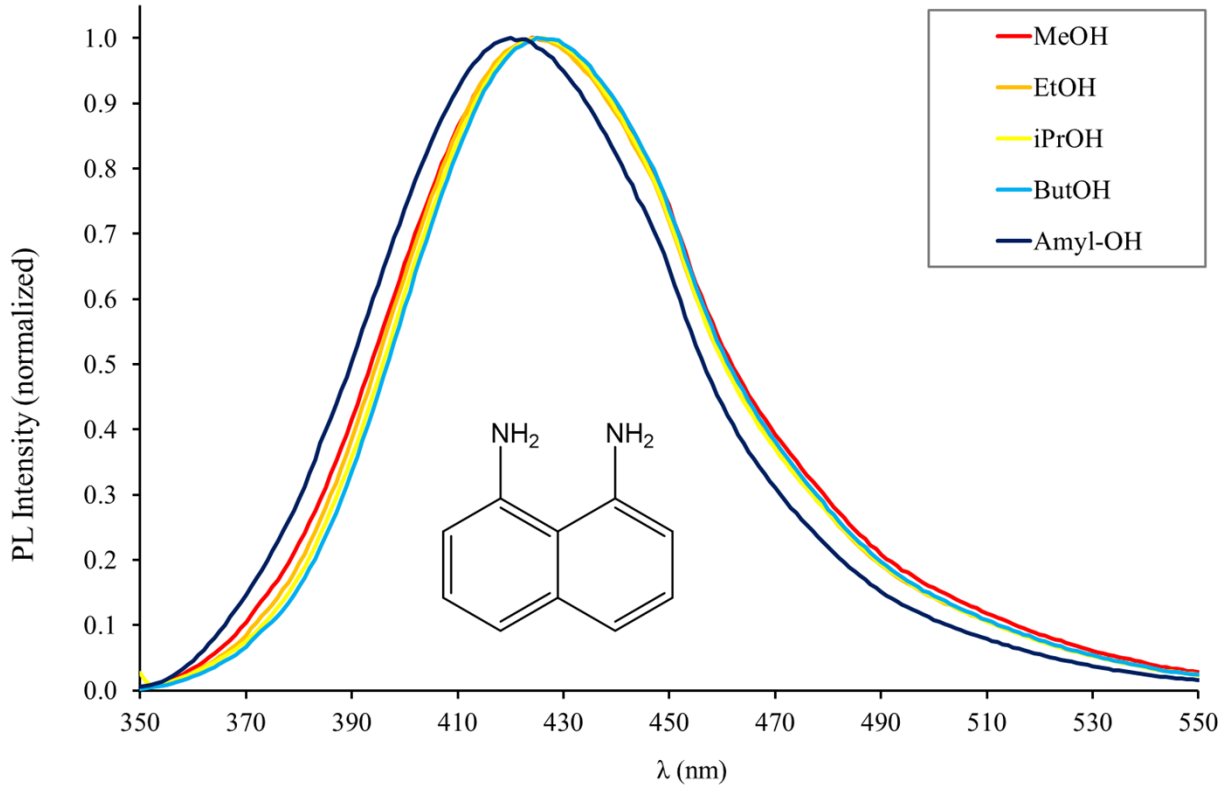


Figure S6. Normalized steady-state fluorescence spectra of 1,5-DAN recorded in various primary alcohols. ([dye] = 1.13×10^{-5} M, T=20 ºC).

Investigation of the solvatochromic behavior of 1,5-DAN and 1,8-DAN

To study the solvatochromic effect of 1,5- and 1,8-DAN in solvents of different polarity we used Reichardt's method, i.e. we plotted the fluorescence emission maxima (ν_{Em}) as a function of the empirical solvent polarity parameter $E_T(30)$ [DOI: 10.1021/cr00032a005], which are presented in Figure S7a and b. It is evident from the figure that in both cases the correlation is linear between the fluorescence emission maximum and $E_T(30)$. It can be surmised from the corresponding slopes that 1,5-DAN has a larger solvatochromic shift (72 $kcal^{-1}cm^{-1}mol$), while this value is slightly lower for the 1,8-DAN (65 $kcal^{-1}cm^{-1}mol$). To account for the specific solvent-dye interactions, i.e. to quantify the solvent effect on the solvatochromic parameters such as emission maxima, and Stokes shifts, multiple linear regression (MLR) analysis employing the Catalan scale [DOI: 10.1021/jp8095727], were used according to the equation:

$$y = y_0 + a_{SA}SA + b_{SB}SB + c_{SP}SP + d_{SdP}SdP \quad (1)$$

where y_0 is the property of the substance of interest (e.g., emission maximum and Stokes shift) in the absence of solvent, for example, in the gas phase. SA is the quantitative empirical measure of the ability of bulk solvent to act as a hydrogen-bond donor towards a solute. SB is the quantitative empirical measure of the ability of a bulk solvent to act as a hydrogen-bond acceptor or electron-pair donor towards a solute, forming a solute-to-solvent hydrogen bond or a solvent-to-solute coordinative bond, respectively. SP and SdP are the solvent polarizability and dipolarity parameters, respectively, determined using reference dye molecules. a, b, c and d are the corresponding coefficients and their inclusion in the equation indicates the dependence of the property under investigation upon the respective solvent parameter. The results are presented in Figure S7c-d and in Table S2. The values of solvatochromic parameters are collected in Table S3.

As seen in Fig.S7b the Catalán equation describes perfectly the specific interactions and based on the data of Table S2 the HB-donor ability (large a coefficient) of the solvent has the largest effect on the solvatochromic behavior, but the effect of solvent polarity is also pronounced.

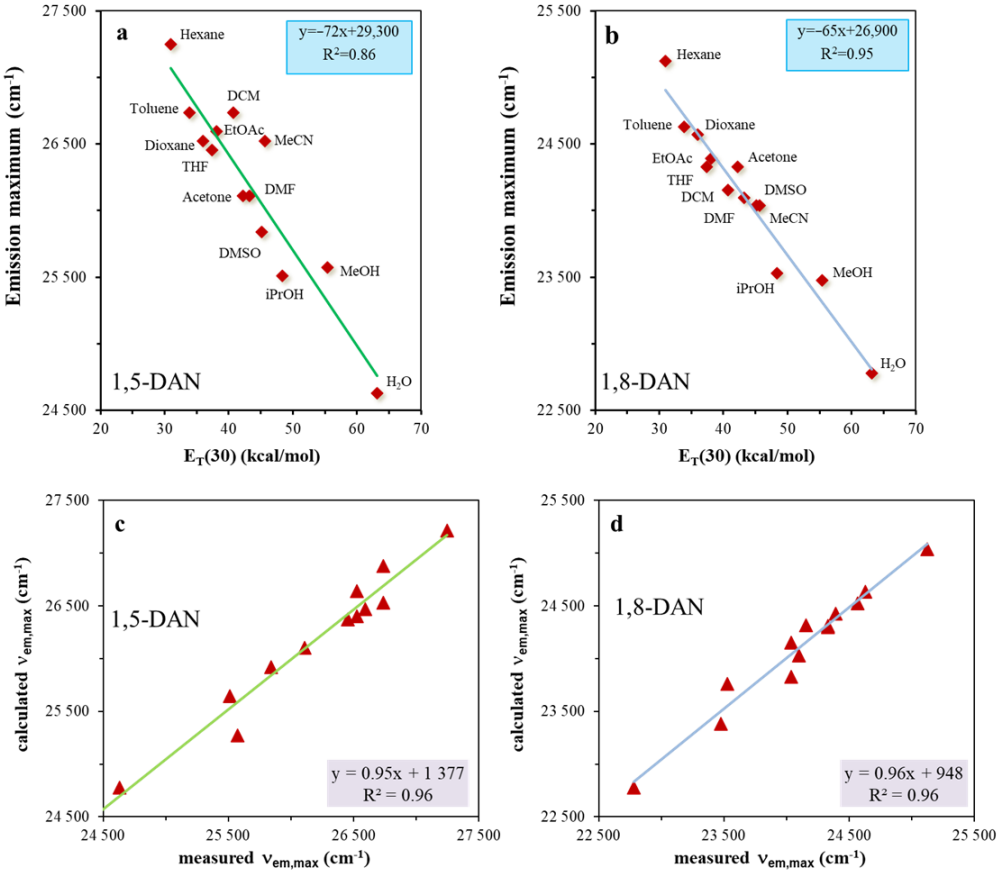


Figure S7. Variation of the fluorescence emission maximum with the empirical solvent polarity parameter $E_T(30)$ (**a**,**b**) and the Catalán (**c**,**d**) plots for the 1,5- and 1,8-diaminonaphthalenes.

Table S2. Solvent-independent correlation coefficients aSA, bSB, cSP and dSdP of the Catalán parameters SA, SB, SP and SdP, respectively, solute property of the reference system (Emission maximum, $\nu_{em,\,max}$ and Stokes-Shift, $\Delta\nu_{ss}$), correlation coefficient (R^2) and number of solvents (n) calculated by multiregression analysis for the solvatochromism of 1,5- and 1-8-diaminonaphthalene.

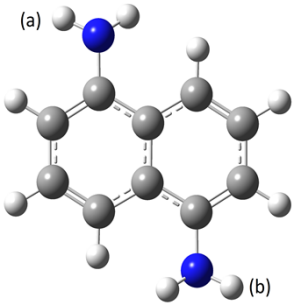
		y_0 (cm^{-1})	a_{SA}	b_{SB}	c_{SP}	d_{SdP}	R^2	n
1,5-DAN	$\nu_{em,ma}$	27724	-1781	-816	-753	-524	0.96	13
	x							
	$\Delta\nu_{ss}$	4641	3398	409	-1038	-1298	0.96	13
1,8-DAN	$\nu_{em,ma}$	25852	-1562	-485	-1280	-536	0.96	13
	x							
	$\Delta\nu_{ss}$	3856	3684	983	-174	41	0.96	13

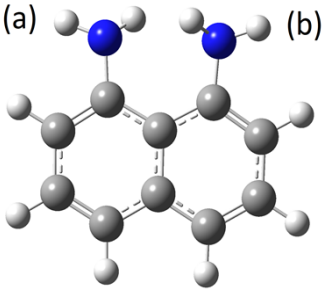
Table S3. The SP, SdP, SA and SB solvent parameters used for constructing Figure 1g,h (Figure S7) using the Catalán equation. *SA* is the quantitative empirical measure of the ability of bulk solvent to act as a hydrogen-bond donor towards a solute. *SB* is the quantitative empirical measure of the ability of a bulk solvent to act as a hydrogen-bond acceptor or electron-pair donor towards a solute, forming a solute-to-solvent hydrogen bond or a solvent-to-solute coordinative bond, respectively. *SP* and *SdP* are the solvent polarizability and dipolarity parameters, respectively. The values were taken from ref.:

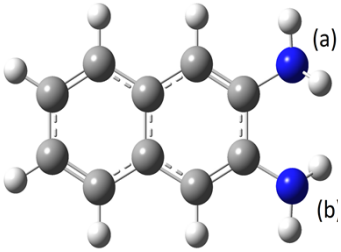
J. Catalán, *J. Phys. Chem. B* **2009**, *113*, 5951–5960.

No	Solvent	SP	SdP	SA	SB
1	Hexane	0.616	0.000	0.000	0.056
2	Cyclohexane	0.683	0.000	0.000	0.073
3	Toluene	0.782	0.284	0.000	0.128
4	1,4-dioxane	0.737	0.312	0.000	0.444
5	Tetrahydrofuran (THF)	0.714	0.634	0.000	0.591
6	Ethyl acetate	0.656	0.603	0.000	0.542
7	Dichloromethane	0.761	0.769	0.040	0.178
8	Chloroform	0.783	0.614	0.047	0.071
9	Acetone	0.651	0.907	0.000	0.475
10	Pyridine	0.842	0.761	0.033	0.581
11	Acetonitrile	0.645	0.974	0.044	0.286
12	Dimethyl formamide (DMF)	0.759	0.977	0.031	0.613
13	Dimethyl sulfoxide (DMSO)	0.830	1.000	0.072	0.647
14	2-propanol	0.633	0.808	0.283	0.830
15	Methanol	0.608	0.904	0.605	0.545
16	Water	0.681	0.997	1.062	0.025

Table S4. The ground (S_0) and excited state (S_1) geometrical and optical properties of DANS calculated on B3LYP/6-311++G(2d,2p) level in DMSO. Numbers in red represent experimental results.







		1,5-DAN		1,8-DAN		2,3-DAN	
		S_0	S_1	S_0	S_1	S_0	S_1
Implicit solvent	**Bond length (Angstrom)**						
	$-NH_2$ (a)	1.396	1.380	1.404	1.344	1.402	1.428
	$-NH_2$ (b)	1.397	1.380	1.404	1.450	1.402	1.348
	abs (nm)	333 (351)	399 (387)	337 (355)	423 (416)	313	380
	Osc. Str	0.1989	0.3133	0.1375	0.1583	0.1384	0.1934
	NH_2 angle (a)	340	348	338	328	338	331
	NH_2 angle (b)	340	348	338	360	338	359
Explicit solvent	**Bond length (Angstrom)**						
	$-NH_2$ (a)	1.384	1.372	1.392	1.413	1.395	1.409
	$-NH_2$ (b)	1.386	1.366	1.393	1.357	1.395	1.349
	abs (nm)	344	411	339	406	328	379
	Osc. Str	0.2647	0.3621	0.1875	0.2274	0.2107	0.2961
	NH_2 angle (a)	347	354	340	335	340	335
	NH_2 angle (b)	346	358	340	359	340	360

Theoretical results

Theoretical calculations were carried out by Gaussian16 software [1], using the standard convergence criteria given as default. Optimization and vibrational frequencies were carried out by the B3LYP method [2,3] using the 6-311++G(2d,2p) basis set and the IEFPCM method for implicit solvent model. Thermodynamic functions were computed at 298.15 K. For wavelength prediction, the vertical excitation was modelled by the TD-B3LYP/6-311++G(2d,2p)//PCM(solvent)[4] level of theory using the geometries optimized at B3LYP/6-311++G(2d,2p)//PCM(solvent). The emission wavelengths were calculated after optimization using geometries provided by

TD-B3LYP/6-311++G(2d,2p)//PCM(solvent).

Ref:

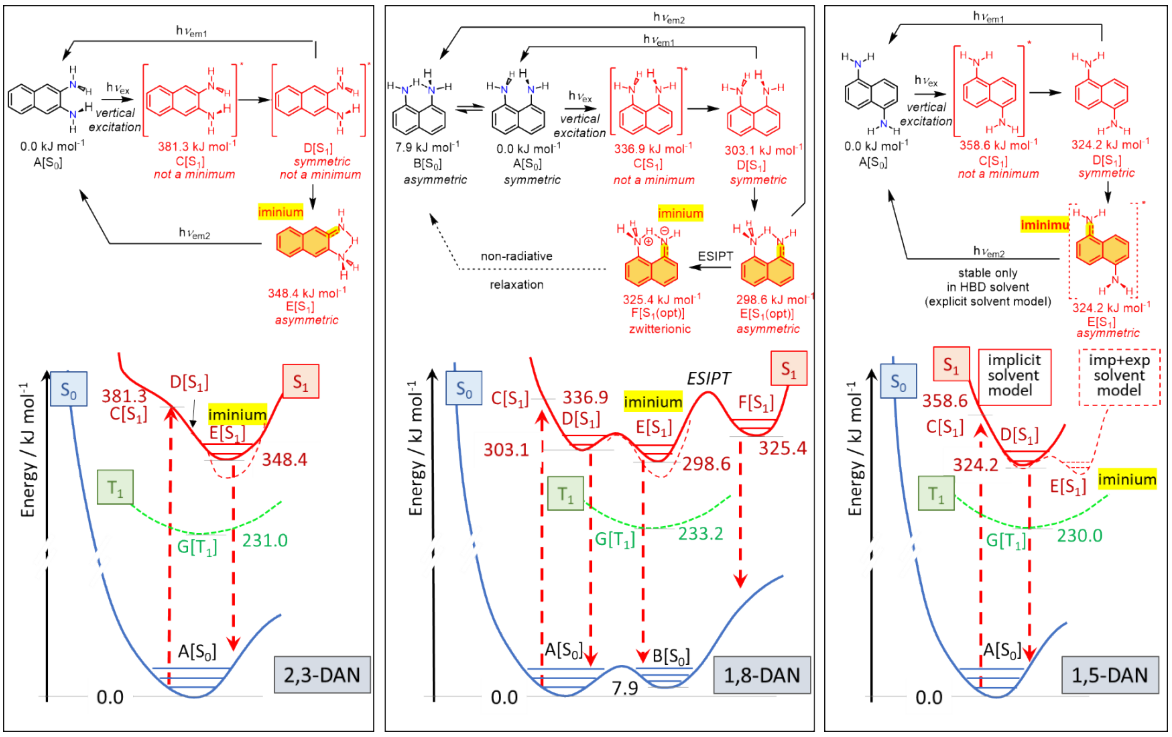
1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V Ortiz, J. Cioslowski and D. J. Fox, Gaussian Inc Wallingford CT, 2016.

2 Y. Zhao and D. G. Truhlar, Theor. Chem. Acc., 2008, 120, 215–241.

3 A. D. Becke, J. Chem. Phys., 1993, 98, 5648–5652.

4 J. Tomasi, B. Mennucci and R. Cammi, Chem. Rev., 2005, 105, 2999–3094.

A)



In the case of 2,3-DAN, the symmetrical ground state form (A[S_0]) undergoes a structural rearrangement upon excitation and the subsequent relaxation (C[S_1]→E[S_1]), resulting asymmetrical structure, skipping the symmetrical state of D[S_1]. At state E[S_1], one of the amino groups form an electron withdrawing quasi iminium group (sp^2), which makes strong HB with another sp^3 amino group (Figure S8A). The vertical excitation of 2,3-DAN A[S_0]→C[S_1] exhibits a single dominant excitation such as HOMO→LUMO (313 nm; f=0.1384).

B)

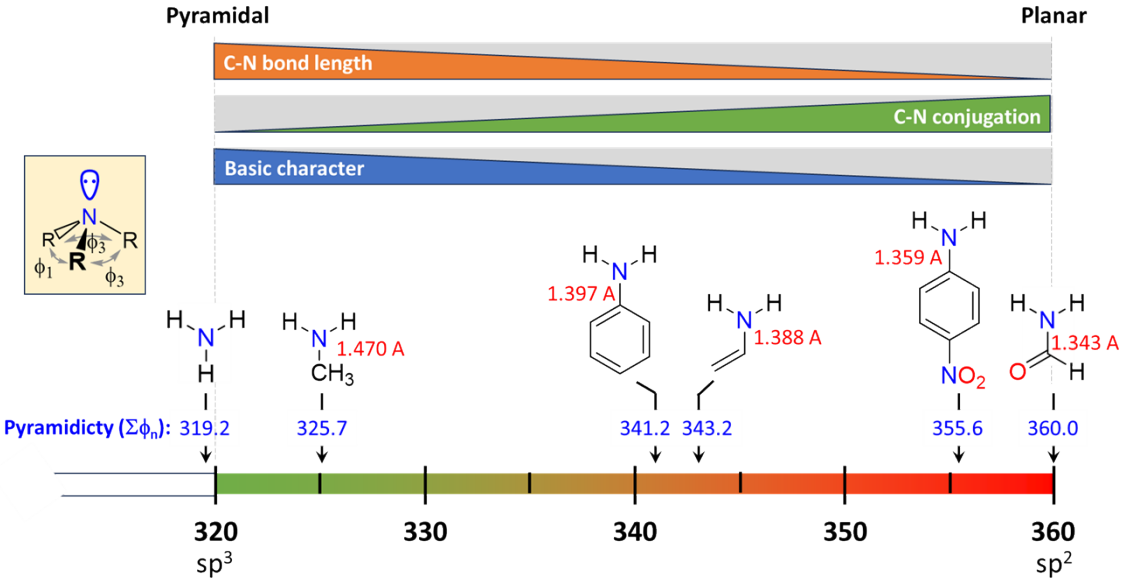


Figure S8. A) The calculated photochemical mechanisms and the corresponding potential energy surfaces (PES) of the ground (blue line, S_0), excited (red line, S_1) and triplet states (green line, T_1) of 2,3-DAN, 1,8-DAN and 1,5-DAN computed at B3LYP/6-311++G(2d,2p)/PCM(DMSO) at S_0 state and TD-B3LYP/6-311++G(2d,2p)/PCM(DMSO) at S_1 state.
B) Definition of Pyramidicity explaind by various amine derivatives as examples.

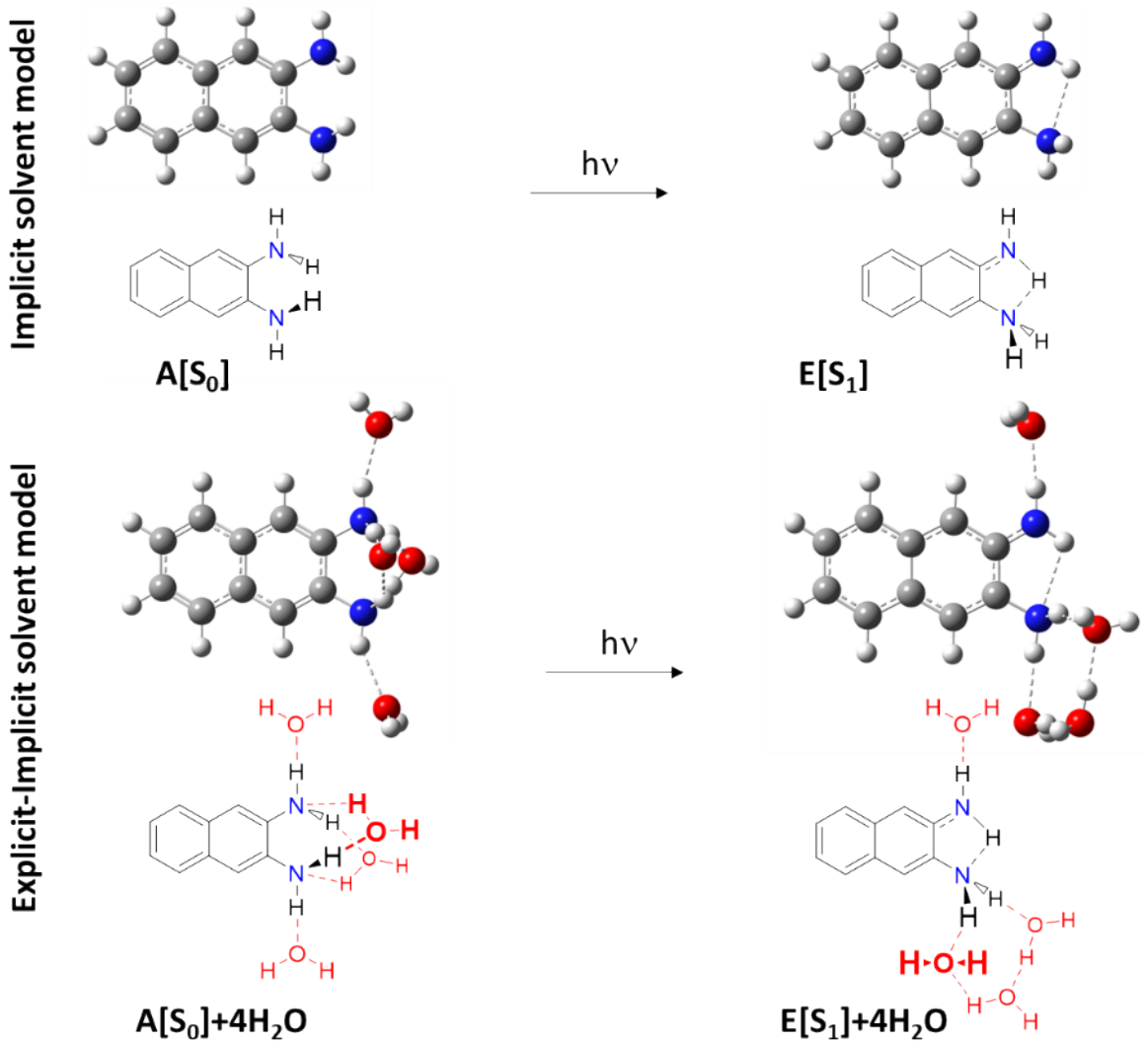


Fig. S9. 3D geometries and 2D representations of 2,3-DAN at S_0 and S_1 states.

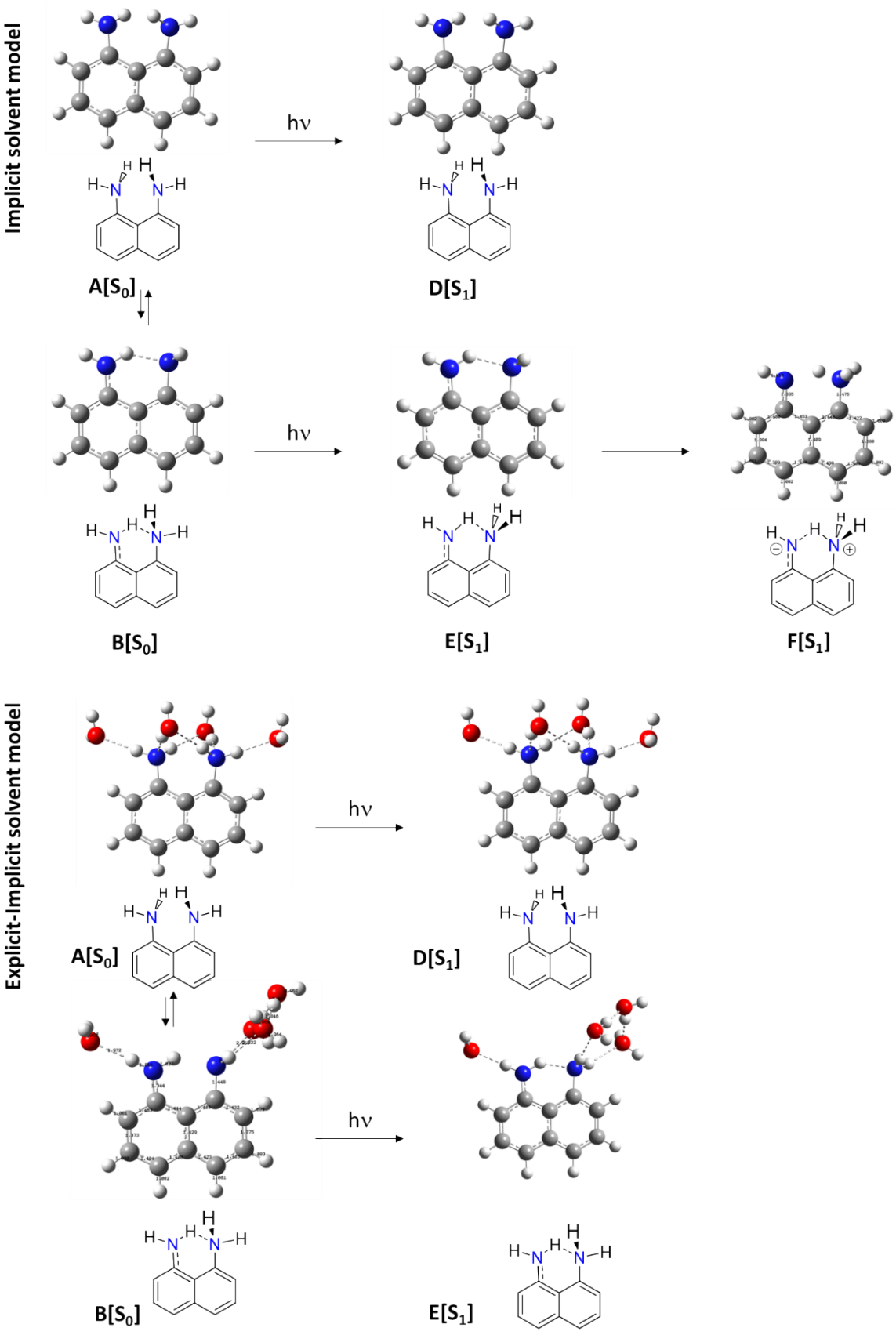


Fig. S10. Various 3D geometries and 2D representations of 1,8-DAN at S_0 and S_1 states.

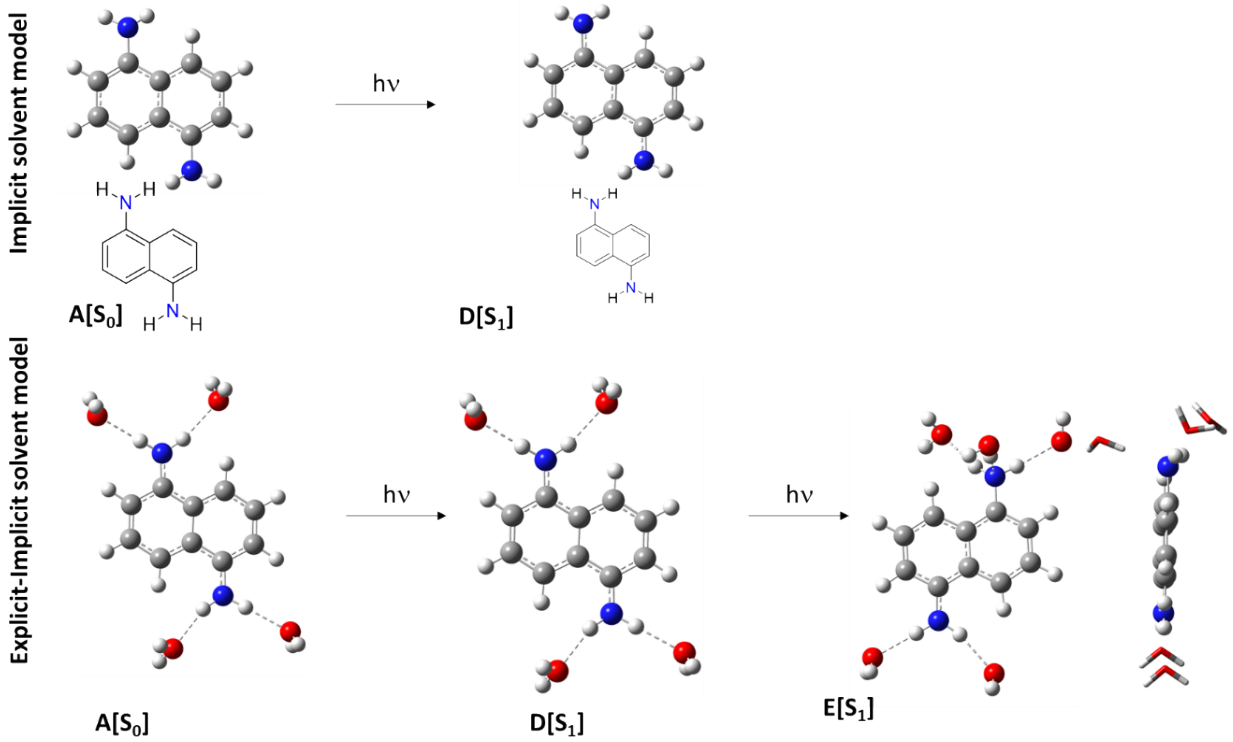


Fig. S11. Various 3D geometries and 2D representations of 1,5-DAN at S_0 and S_1 states.

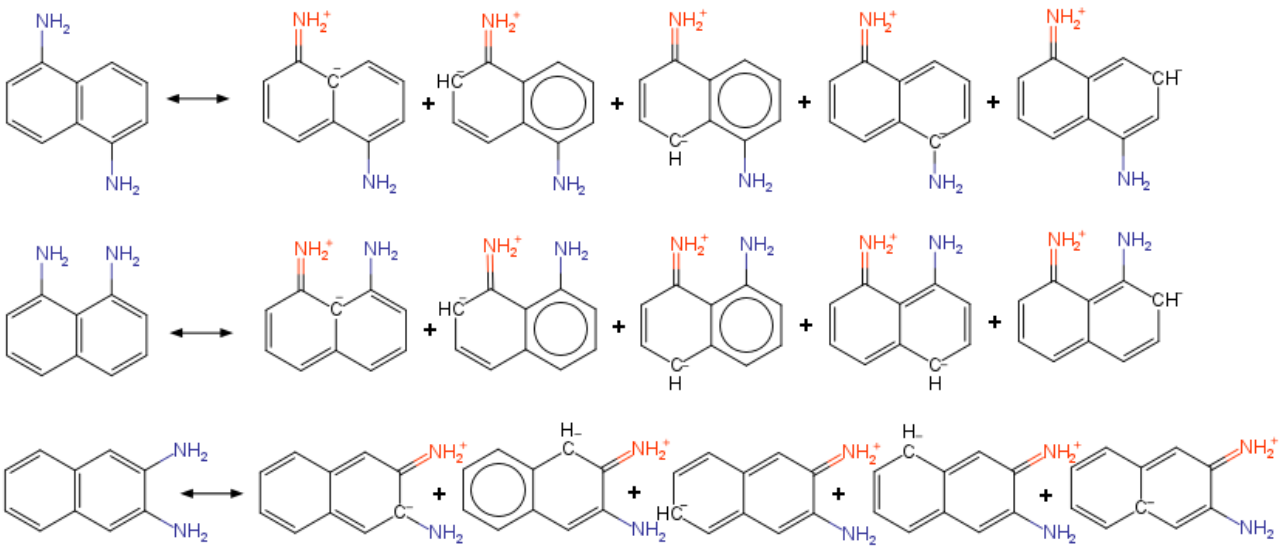


Figure S12. The suggested resonance structures of 1,5-DAN, 1,8-DAN and 2,3-DAN respectively calculated by Marvinsketch software.

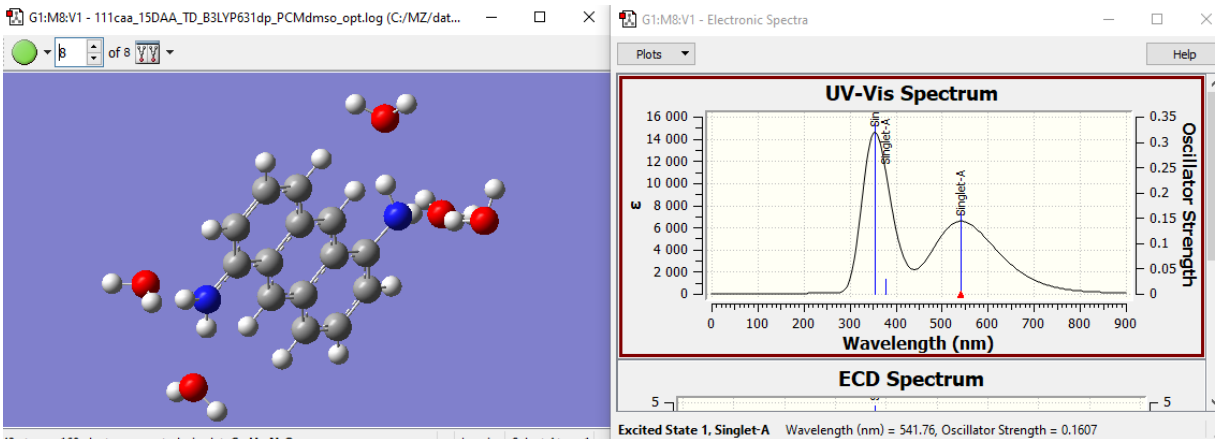


Fig. S13. The optimized structure and emission spectrum of 1,5-diaminoanthracene in S_1 state, calculated using the implicit-explicit solvent model.

The solvatochromic behavior of 1,5-diaminoanthracene is described in:

Nagy, M.; Fiser, B.; Szőri, M.; Vanyorek, L.; Viskolcz, B. Optical Study of Solvatochromic Isocyanoaminoanthracene Dyes and 1,5-Diaminoanthracene. *Int. J. Mol. Sci.* **2022**, *23*, 1315. https://doi.org/10.3390/ijms23031315

Raw computational data

Table S5. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYP/6-311++G(2d,2p) basis set with the consideration of PCM solvent method using the parameter set of water for compound 2,3-DAN.

Conformer	Filename	E	ZPE	U	H	G	S
S0	0001aaa_23-diaminonaftalin_B3lyp6311++2d2pPCMdmso.log	-496.77131495	-496.590541	-496.580991	-496.580047	-496.624715	94.013
S0	0001aaf_23-diaminonaftalin_B3lyp6311++2d2pPCMw.log	-496.77147971	-496.590708	-496.581161	-496.580217	-496.624880	94.002
S0	0001aam_23-diaminonaftalin_+4HOH_B3lyp6311++2d2p_PCMw.log	-802.31368346	-802.034657	-802.010743	-802.009799	-802.090987	170.876
S1	0001baf_23-diaminonaftalin_TD_B3lyp6311++2d2pPCMw_spopt.log	-496.75861401					
S1	0001caa_23-diaminonaftalin_TD_B3lyp6311++2d2pPCMdmso_opt.log	-496.75832374					
S0	0011aaa_23-diaminonaftalin_+4HOH_B3lyp6311++2d2p_PCMw.log	-802.66689847	-802.391330	-802.366773	-802.365829	-802.451235	179.751
S0	0021cba_23-diaminonaftalin_+3DMSO_B3lyp6311++2d2pPCMdmso_f.log	-2709.99251136	-2709.491064	-2709.450887	-2709.449943	-2709.578419	270.401

Table S6. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYP/6-311++G(2d,2p) basis set with the consideration of PCM solvent method using the parameter set of water for compound 1,8-DAN.

Conformer	Filename	E	ZPE	U	H	G	S
S0	0401aaa_1_8_DAN_b3lyp6311++2d2p_PCMdmso_NOSYMM.log	-496.76106693	-496.580585	-496.570942	-496.569998	-496.614805	94.305
S1	0401aaa_1_8_DAN_TD_b3lyp6311++2d2p_PCMdmso_NOSYMM_opt.log	-496.74818804					
S0	0401aabm_1_8_DAN_b3lyp6311++2d2p_PCMw_NOSYMM.log	-496.76423303	-496.583066	-496.573608	-496.572664	-496.617218	93.771
S1	0401aabm_1_8_DAN_TD_b3lyp6311++2d2p_PCMw_NOSYMM_opt.log	-496.75428513					
S1	0401aac_1_8_DAN_protontransfer_TD_b3lyp6311++2d2p_PCMdmso_NOSYMM_opt.log	-496.70995372					
S1	0401aacm_1_8_DAN_protontransfer_TD_b3lyp6311++2d2p_PCMw_NOSYMM_opt.log	-496.71041959					
S1	0401acaa_1_8_DAN_b3lyp6311++2d2p_PCMwater.log	-496.75695063	-496.577880	-496.569228	-496.568283	-496.611337	90.614
S1	0401acam_1_8_DAN_TD_b3lyp6311++2d2p_PCMw_opt.log	-496.74834035					
S1	0401acb_1_8_DAN_TD_b3lyp6311++2d2p_PCMdmso_opt.log	-496.75419098					
S1	0401ada_1_8_DAN_b3lyp6311++2d2p_PCMdmso_TRIPLET.log	-496.67518396					
T1	0401facm_1_8_DAN_protontransfer_b3lyp6311++2d2p_PCMdmso_NOSYMM_opt_TRIPLET.log	-496.65318076					
S0	0406dab_1_8_DAN+4DMSO_b3lyp6311++2d2p_PCMdmso_NOSYMM.log	-2709.98287096	-2709.481795	-2709.441346	-2709.440402	-2709.569073	270.812
S1	0406qbb_1_8_DAN_HB_+4HOH_TD_b3lyp6311++2d2pdp_PCMw_NOSYMM_optsp.log	-802.64467639					
S1	0406qcb_1_8_DAN+4HOH_TD_sym_b3lyp6311++2d2p_PCMw_NOSYMM_jo_spopt.log	-802.64763954					

Table S7. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYP/6-311++G(2d,2p) basis set with the consideration of PCM solvent method using the parameter set of water for compound 1,5-DAN.

Conformer	Filename	E	ZPE	U	H	G	S
S0	0402aaa_1_5_DAN_b3lyp6311++2d2p_PCMdmso.log	-496.76850128	-496.587860	-496.578189	-496.577245	-496.622127	94.464
T1	0402ada_1_5_DAN_b3lyp6311++2d2p_PCMdmso_TRIPLET.log	-496.68081920					
S1	0412aaam_1_5_DAN_b3lyp6311++2d2p_PCMw_NOsymm.log	-496.76874662	-496.588037	-496.578401	-496.577457	-496.622238	94.251
S1	0412baaa_1_5_DAN_TD_b3lyp6311++2d2p_PCMdmso_NOsymm_opt.log	-496.75923322					
S1	0412baaam_1_5_DAN_TD_b3lyp6311++2d2p_PCMw_NOsymm_opt.log	-496.75941823					
S0	0413caa_1_5_DAN_4DMSO_b3lyp6311++2d2p_PCMdmso.log	-2709.99009880	-2709.489343	-2709.448603	-2709.447658	-2709.579619	277.734
S1	0413cca_1_5_DAN_4DMSO_TD_b3lyp6311++2d2p_PCMdmso_opt.log	-2709.98151025					
S1	0413qdab_1_5_DAN_5HOH_TD_b3lyp6311++2d2p_PCMw_spopt_assym.log	-879.12288478					

The xyz coordinates of computed geometries

0001aaa_23-diaminonaftalin_B3lyp6311++2d2pPCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.154866	0.706191	-0.010645
2	6	0	1.966288	1.397699	-0.022022
3	6	0	0.724679	0.714220	-0.011795
4	6	0	0.724660	-0.714224	0.011744
5	6	0	1.966305	-1.397678	0.022031
6	6	0	3.154862	-0.706137	0.010713
7	1	0	-0.522340	2.477538	-0.004569
8	1	0	4.094046	1.242694	-0.018323
9	1	0	1.965904	2.480384	-0.038029
10	6	0	-0.517767	1.394252	-0.008911
11	6	0	-0.517730	-1.394298	0.008825
12	1	0	1.965960	-2.480361	0.038068
13	1	0	4.094045	-1.242636	0.018448
14	6	0	-1.715098	-0.717426	-0.004939
15	6	0	-1.715036	0.717331	0.004905
16	1	0	-0.522240	-2.477590	0.004376
17	7	0	-2.952146	-1.374698	0.040559
18	1	0	-3.660597	-0.957994	-0.548340
19	1	0	-2.889945	-2.366211	-0.138044
20	7	0	-2.952351	1.374647	-0.040653
21	1	0	-3.659875	0.958703	0.550035
22	1	0	-2.889648	2.366243	0.137610

0001aaf_23-diaminonaftalin_B3lyp6311++2d2pPCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.154918	-0.706210	-0.010572
2	6	0	-1.966322	-1.397736	-0.021769
3	6	0	-0.724668	-0.714254	-0.011635
4	6	0	-0.724659	0.714264	0.011615
5	6	0	-1.966345	1.397716	0.021722
6	6	0	-3.154919	0.706159	0.010500
7	1	0	0.522389	-2.477539	-0.004106
8	1	0	-4.094070	-1.242718	-0.018189
9	1	0	-1.965956	-2.480401	-0.037575
10	6	0	0.517751	-1.394278	-0.008597
11	6	0	0.517721	1.394324	0.008637
12	1	0	-1.966015	2.480380	0.037535
13	1	0	-4.094078	1.242657	0.018098
14	6	0	1.715152	0.717454	-0.004934
15	6	0	1.715118	-0.717379	0.005001
16	1	0	0.522319	2.477587	0.004110
17	7	0	2.952118	1.374785	0.041194
18	1	0	3.661004	0.958242	-0.547436
19	1	0	2.890004	2.366357	-0.137538
20	7	0	2.952261	-1.374731	-0.041251
21	1	0	3.660517	-0.958914	0.548717
22	1	0	2.889769	-2.366399	0.136972

0001aam_23-diaminonaftalin_+4HOH_B3lyp6311++2d2p_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.215672	-0.705421	-0.027776
2	6	0	-3.032215	-1.394522	-0.055558
3	6	0	-1.792760	-0.708462	-0.028647
4	6	0	-1.792498	0.709072	0.029112
5	6	0	-3.031706	1.395579	0.056033
6	6	0	-4.215413	0.706902	0.028265
7	1	0	-0.543499	-2.475409	-0.054350
8	1	0	-5.155213	-1.239962	-0.048676
9	1	0	-3.027850	-2.476359	-0.097702
10	6	0	-0.552197	-1.392324	-0.038890
11	6	0	-0.551678	1.392472	0.039337
12	1	0	-3.026963	2.477415	0.098178
13	1	0	-5.154755	1.241792	0.049174
14	6	0	0.638791	0.716276	0.006374
15	6	0	0.638523	-0.716569	-0.005921
16	1	0	-0.542592	2.475557	0.054761
17	7	0	1.880540	1.384772	0.045742
18	1	0	2.520905	1.033801	-0.662754
19	1	0	1.767981	2.388791	-0.064200
20	7	0	1.880005	-1.385548	-0.045399
21	1	0	2.520562	-1.035080	0.663160
22	1	0	1.767051	-2.389559	0.064179
23	8	0	1.419048	-4.407784	0.192287
24	1	0	0.900676	-4.717233	0.939881
25	1	0	1.029723	-4.836210	-0.574698
26	8	0	1.421008	4.407008	-0.193160
27	1	0	0.902550	4.716802	-0.940551
28	1	0	1.032062	4.835448	0.574012
29	8	0	3.112156	-0.252716	-2.343736
30	1	0	2.760389	-0.831111	-1.638310
31	8	0	3.115342	0.252528	2.343357
32	1	0	4.034122	0.508900	2.450627
33	1	0	2.762305	0.830047	1.637855
34	1	0	4.029247	-0.512518	-2.456939

0001baf_23-diaminonaftalin_TD_B3lyp6311++2d2pPCMw_spopt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.162171	-0.733070	-0.020597
2	6	0	-1.931560	-1.425784	-0.022655
3	6	0	-0.703244	-0.728738	-0.005843
4	6	0	-0.751221	0.719023	0.014324
5	6	0	-2.001807	1.382843	0.017245
6	6	0	-3.209234	0.654273	0.000282
7	1	0	0.576117	-2.465100	0.022832
8	1	0	-4.083053	-1.301920	-0.035790
9	1	0	-1.926379	-2.507469	-0.033726
10	6	0	0.559756	-1.381923	0.016156
11	6	0	0.469872	1.410512	0.037691
12	1	0	-2.017062	2.464933	0.033074
13	1	0	-4.158476	1.170872	0.002618
14	6	0	1.723865	0.717796	0.007805
15	6	0	1.778708	-0.690845	0.028204
16	1	0	0.483120	2.492274	0.069263
17	7	0	2.859151	1.442269	-0.053602
18	1	0	3.737242	0.963174	-0.183258
19	1	0	2.838107	2.445637	-0.124163
20	7	0	3.058276	-1.319666	-0.034914
21	1	0	3.494254	-1.421554	0.876775
22	1	0	2.996349	-2.243580	-0.443678

0001caa_23-diaminonaftalin_TD_B3lyp6311++2d2pPCMdmso_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.162132	-0.733288	-0.020429
2	6	0	-1.931479	-1.425813	-0.022421
3	6	0	-0.703272	-0.728668	-0.005566
4	6	0	-0.751481	0.718993	0.014260
5	6	0	-2.001762	1.382558	0.017078
6	6	0	-3.209354	0.653946	0.000249
7	1	0	0.576201	-2.464891	0.022569
8	1	0	-4.082887	-1.302334	-0.035562
9	1	0	-1.926230	-2.507493	-0.033455
10	6	0	0.559777	-1.381712	0.016157
11	6	0	0.469834	1.410810	0.037111
12	1	0	-2.017187	2.464645	0.032657
13	1	0	-4.158540	1.170609	0.002464
14	6	0	1.723459	0.718240	0.007538
15	6	0	1.778716	-0.690562	0.027572
16	1	0	0.482800	2.492601	0.068124
17	7	0	2.859245	1.442110	-0.052493
18	1	0	3.736505	0.960887	-0.180442
19	1	0	2.839079	2.445364	-0.124296
20	7	0	3.059313	-1.318378	-0.033573
21	1	0	3.484675	-1.437829	0.881064
22	1	0	3.001846	-2.234704	-0.459950

0011aaa_23-diaminonaftalin_+4HOH_B3lyp6311++2d2p_PCMw.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.313721	0.706338	0.025665
2	6	0	-3.125948	1.397767	0.051463
3	6	0	-1.884586	0.713647	0.026808
4	6	0	-1.884706	-0.713354	-0.026850
5	6	0	-3.126183	-1.397266	-0.051487
6	6	0	-4.313839	-0.705638	-0.025671
7	1	0	-0.634985	2.476234	0.043993
8	1	0	-5.253122	1.242026	0.044715
9	1	0	-3.125216	2.479730	0.090100
10	6	0	-0.642337	1.393666	0.033555
11	6	0	-0.642571	-1.393580	-0.033612
12	1	0	-3.125632	-2.479229	-0.090124
13	1	0	-5.253330	-1.241169	-0.044706
14	6	0	0.554006	-0.716856	-0.002819
15	6	0	0.554126	0.716743	0.002748
16	1	0	-0.635397	-2.476149	-0.044055
17	7	0	1.795888	-1.390840	-0.034673
18	1	0	2.444397	-1.035746	0.662676
19	1	0	1.697221	-2.396487	0.078612
20	7	0	1.796124	1.390517	0.034600
21	1	0	2.444554	1.035337	-0.662782
22	1	0	1.697623	2.396183	-0.078672
23	8	0	1.529590	4.461696	-0.223862
24	1	0	1.636507	4.815198	-1.113209
25	1	0	2.154771	4.956187	0.316468
26	8	0	3.227324	-0.428212	-2.327484
27	1	0	2.781967	-0.917807	-1.601699
28	1	0	4.153773	-0.681992	-2.276387
29	8	0	3.227422	0.427721	2.327437
30	1	0	2.782131	0.917331	1.601623
31	1	0	4.153910	0.681351	2.276303
32	8	0	1.528580	-4.461894	0.223905
33	1	0	1.633187	-4.815129	1.113633
34	1	0	2.154790	-4.956899	-0.314759

0021cba_23-diaminonaftalin_+3DMSO_B3lyp6311++2d2pPCMdmso_f.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.257127	6.360835	0.181372
2	6	0	0.984108	5.223443	0.450586
3	6	0	0.451491	3.935822	0.192333
4	6	0	-0.863256	3.833107	-0.359301
5	6	0	-1.586615	5.022583	-0.624366
6	6	0	-1.042662	6.259272	-0.361065
7	1	0	2.182120	2.817642	0.838906
8	1	0	0.679972	7.335544	0.385010
9	1	0	1.981206	5.301143	0.866418
10	6	0	1.175845	2.745220	0.444427
11	6	0	-1.397072	2.544260	-0.603448
12	1	0	-2.583647	4.944476	-1.040352
13	1	0	-1.609783	7.156621	-0.569548
14	6	0	-0.688347	1.391824	-0.336072
15	6	0	0.651612	1.496375	0.184300
16	1	0	-2.402163	2.460116	-0.998686
17	7	0	-1.202708	0.126268	-0.608834
18	1	0	-0.975043	-0.592972	0.071432
19	1	0	-2.199328	0.115142	-0.806918
20	7	0	1.353674	0.326827	0.466767
21	1	0	1.232347	-0.427532	-0.201741
22	1	0	2.344035	0.469853	0.647682
23	16	0	-5.067713	-0.680293	-0.046670
24	8	0	-4.197427	-0.199084	-1.204459
25	16	0	1.444901	-2.925330	-2.452005
26	8	0	2.109953	-2.028759	-1.411423
27	16	0	5.475172	-0.173934	0.338914
28	8	0	4.349340	0.618381	0.997331
29	6	0	0.228265	-3.935918	-1.554843
30	1	0	-0.368074	-4.485438	-2.280350
31	1	0	0.794093	-4.629980	-0.938865
32	1	0	-0.388919	-3.290158	-0.934158
33	6	0	0.278400	-1.869368	-3.362472
34	1	0	0.878136	-1.181929	-3.953365
35	1	0	-0.320299	-2.498060	-4.018270
36	1	0	-0.337627	-1.327447	-2.646724
37	6	0	5.119258	-1.930382	0.649537
38	1	0	5.868499	-2.527992	0.133713
39	1	0	5.199278	-2.080537	1.722782
40	1	0	4.118088	-2.157577	0.290102
41	6	0	5.133732	-0.173184	-1.447293
42	1	0	5.214353	0.858376	-1.779271
43	1	0	5.891214	-0.781234	-1.938263
44	1	0	4.135617	-0.571035	-1.619228
45	6	0	-4.688750	-2.442508	0.177482
46	1	0	-3.664064	-2.495468	0.540916
47	1	0	-5.374099	-2.852019	0.917179
48	1	0	-4.793849	-2.950003	-0.779082
49	6	0	-6.745540	-0.859758	-0.721237
50	1	0	-7.381821	-1.302243	0.042255
51	1	0	-7.095335	0.139700	-0.964763
52	1	0	-6.705609	-1.482305	-1.612124
53	16	0	-1.004117	-2.433466	2.785050
54	8	0	-1.391668	-2.287350	1.316593
55	6	0	0.753590	-2.899228	2.806806
56	1	0	1.095079	-2.914440	3.839714
57	1	0	0.820170	-3.895158	2.377757
58	1	0	1.314092	-2.181065	2.213319
59	6	0	-0.815076	-0.745775	3.436588
60	1	0	-1.804022	-0.295655	3.431493
61	1	0	-0.440311	-0.809530	4.456059
62	1	0	-0.131188	-0.197358	2.792458

0401acaa_1_8_DAN_b3lyp6311++2d2p_PCMwater.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.492326	-1.165989	-0.000037
2	6	0	1.335414	-1.904206	-0.000027
3	6	0	0.079008	-1.248173	-0.000007
4	6	0	-0.001503	0.189625	-0.000003
5	6	0	1.243421	0.932310	-0.000020
6	6	0	2.447726	0.233495	-0.000032
7	1	0	-1.027064	-3.095569	0.000011
8	1	0	3.454590	-1.661142	-0.000048
9	1	0	1.361932	-2.985053	-0.000029
10	6	0	-1.112123	-2.016752	0.000017
11	6	0	-1.305835	0.780793	0.000028
12	1	0	3.371124	0.798473	-0.000041
13	6	0	-2.432346	-0.014285	0.000039
14	6	0	-2.343252	-1.417438	0.000037
15	1	0	-3.403383	0.462858	0.000051
16	1	0	-3.245654	-2.013467	0.000049
17	7	0	1.260469	2.299360	-0.000038
18	1	0	2.136709	2.787335	0.000080
19	1	0	0.378296	2.791174	0.000102
20	7	0	-1.465942	2.225439	0.000041
21	1	0	-2.002422	2.512794	-0.810774
22	1	0	-2.002844	2.512717	0.810603

0401acam_1_8_DAN_TD_b3lyp6311++2d2p_PCMw_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.564018	-1.110874	0.000034
2	6	0	1.368267	-1.847426	0.000028
3	6	0	0.085904	-1.240366	-0.000033
4	6	0	-0.017661	0.184809	-0.000020
5	6	0	1.224215	0.919205	0.000009
6	6	0	2.494744	0.259684	0.000021
7	1	0	-0.989086	-3.122123	-0.000113
8	1	0	3.517892	-1.617058	0.000054
9	1	0	1.416971	-2.928480	0.000066
10	6	0	-1.086740	-2.045977	-0.000090
11	6	0	-1.312697	0.783649	-0.000083
12	1	0	3.387610	0.869464	0.000025
13	6	0	-2.469736	-0.060775	0.000044
14	6	0	-2.360272	-1.431148	0.000035
15	1	0	-3.444869	0.409797	0.000147
16	1	0	-3.253066	-2.043083	0.000129
17	7	0	1.214082	2.264914	-0.000034
18	1	0	2.075298	2.786143	-0.000018
19	1	0	0.295040	2.720311	0.000032
20	7	0	-1.486361	2.222236	0.000027
21	1	0	-2.020002	2.525216	-0.810699
22	1	0	-2.020087	2.525073	0.810756

0401acb_1_8_DAN_TD_b3lyp6311++2d2p_PCMdmso_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.465967	-1.259626	-0.131085
2	6	0	1.226807	-1.943534	-0.063819
3	6	0	-0.000018	-1.247004	0.000029
4	6	0	0.000006	0.196913	0.000023
5	6	0	1.262710	0.850712	0.072704
6	6	0	2.485710	0.106809	-0.066366
7	1	0	-1.207965	-3.024423	0.099874
8	1	0	3.387054	-1.816917	-0.227623
9	1	0	1.207845	-3.024478	-0.099829
10	6	0	-1.226883	-1.943479	0.063860
11	6	0	-1.262674	0.850749	-0.072699
12	1	0	3.418501	0.654151	-0.104938
13	6	0	-2.485722	0.106892	0.066307
14	6	0	-2.466020	-1.259540	0.131048
15	1	0	-3.418490	0.654273	0.104831
16	1	0	-3.387126	-1.816807	0.227545
17	7	0	1.389152	2.227179	0.243483
18	1	0	2.308125	2.530824	0.529619
19	1	0	0.660795	2.689258	0.768299
20	7	0	-1.389095	2.227176	-0.243497
21	1	0	-0.660474	2.689394	-0.767816
22	1	0	-2.307968	2.530887	-0.529873

0401ada_1_8_DAN_b3lyp6311++2d2p_PCMdmso_TRIPLET.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.470214	-1.263170	0.110668
2	6	0	-1.220713	-1.948495	0.055402
3	6	0	-0.000010	-1.246947	-0.000009
4	6	0	0.000047	0.202828	-0.000001
5	6	0	-1.262597	0.852488	-0.060768
6	6	0	-2.485465	0.094712	0.053055
7	1	0	1.198102	-3.029328	-0.076370
8	1	0	-3.391554	-1.822550	0.189162
9	1	0	-1.197840	-3.029349	0.076007
10	6	0	1.220880	-1.948481	-0.055501
11	6	0	1.262415	0.852575	0.060803
12	1	0	-3.421250	0.638708	0.079438
13	6	0	2.485539	0.094786	-0.052906
14	6	0	2.470216	-1.263070	-0.110595
15	1	0	3.421275	0.638847	-0.079173
16	1	0	3.391575	-1.822458	-0.188995
17	7	0	-1.396259	2.241821	-0.184241
18	1	0	-2.321270	2.536841	-0.459504
19	1	0	-0.690860	2.701270	-0.742114
20	7	0	1.396154	2.241973	0.184054
21	1	0	0.690852	2.701318	0.742206
22	1	0	2.321132	2.536786	0.459764

0402aaa_1_5_DAN_b3lyp6311++2d2p_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.417250	-2.090557	0.002541
2	6	0	-0.060462	-1.876019	0.019965
3	6	0	0.452858	-0.554692	0.008066
4	6	0	-0.452871	0.554673	-0.008119
5	6	0	-1.864235	0.292853	-0.009207
6	6	0	-2.317878	-1.013550	-0.011686
7	1	0	-1.804277	-3.100489	0.014859
8	1	0	0.605444	-2.724714	0.060275
9	6	0	1.864197	-0.292783	0.009175
10	6	0	0.060500	1.876020	-0.019983
11	1	0	-3.383233	-1.205072	-0.011957
12	6	0	1.417244	2.090598	-0.002472
13	6	0	2.317878	1.013517	0.011768
14	1	0	1.804307	3.100511	-0.014762
15	1	0	3.383231	1.205050	0.012188
16	7	0	-2.771683	1.352434	-0.070358
17	1	0	-3.715751	1.097657	0.177111
18	1	0	-2.493693	2.195056	0.407561
19	1	0	-0.605401	2.724710	-0.060338
20	7	0	2.771677	-1.352593	0.070469
21	1	0	2.493859	-2.194503	-0.408925
22	1	0	3.715674	-1.097451	-0.177074

0402ada_1_5_DAN_b3lyp6311++2d2p_PCMdmso_TRIPLET.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.554992	-2.043637	-0.001855
2	6	0	0.136351	-1.863728	-0.043329
3	6	0	-0.436894	-0.579496	-0.014779
4	6	0	0.436894	0.579497	0.014777
5	6	0	1.841505	0.366818	0.008625
6	6	0	2.385019	-0.970322	0.030778
7	1	0	1.959655	-3.046316	-0.000986
8	1	0	-0.485953	-2.744316	-0.101083
9	6	0	-1.841505	-0.366818	-0.008623
10	6	0	-0.136352	1.863729	0.043323
11	1	0	3.459349	-1.095488	0.061924
12	6	0	-1.554992	2.043637	0.001849
13	6	0	-2.385019	0.970321	-0.030780
14	1	0	-1.959656	3.046315	0.000977
15	1	0	-3.459349	1.095487	-0.061926
16	7	0	2.735275	1.425876	0.045160
17	1	0	3.682524	1.203700	-0.218686
18	1	0	2.430238	2.303118	-0.346629
19	1	0	0.485951	2.744318	0.101069
20	7	0	-2.735273	-1.425878	-0.045150
21	1	0	-2.430237	-2.303112	0.346656
22	1	0	-3.682524	-1.203698	0.218693

0406dab_1_8_DAN+4DMSO_b3lyp6311++2d2p_PCMdmso_NOSYMM.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.234133	3.942780	-1.594737
2	6	0	-1.125419	4.690249	-1.288564
3	6	0	0.010953	4.077486	-0.701606
4	6	0	0.016256	2.661216	-0.443071
5	6	0	-1.201245	1.928105	-0.689307
6	6	0	-2.277419	2.576640	-1.284794
7	1	0	1.107201	5.931074	-0.560842
8	1	0	-3.097936	4.409215	-2.050623
9	1	0	-1.098554	5.753011	-1.488389
10	6	0	1.142604	4.866399	-0.373056
11	6	0	1.240052	2.070224	0.040708
12	1	0	-3.179386	2.009606	-1.473412
13	6	0	2.312797	2.895269	0.361504
14	6	0	2.258911	4.282399	0.169754
15	1	0	3.220292	2.437780	0.732633
16	1	0	3.120176	4.885516	0.426735
17	7	0	-1.334538	0.577685	-0.376641
18	1	0	-2.290807	0.242187	-0.436750
19	1	0	-0.904004	0.272076	0.486400
20	7	0	1.387217	0.698252	0.227380
21	1	0	0.931472	0.096009	-0.446952
22	1	0	2.351808	0.414077	0.367958
23	16	0	4.753223	-1.646334	0.468501
24	8	0	4.301648	-0.203254	0.675128
25	16	0	-4.727214	-1.698833	0.213288
26	8	0	-4.184353	-0.556221	-0.640379
27	6	0	-6.521158	-1.732770	-0.078023
28	1	0	-6.666294	-2.033143	-1.112103
29	1	0	-6.968600	-2.465741	0.590082
30	1	0	-6.927930	-0.739155	0.095759
31	6	0	-4.754048	-1.090174	1.924085
32	1	0	-5.243123	-1.836018	2.547758
33	1	0	-3.715166	-0.966747	2.224661
34	1	0	-5.288195	-0.142854	1.952701
35	6	0	4.524728	-2.006273	-1.297031
36	1	0	4.929189	-2.995760	-1.501164
37	1	0	3.453233	-1.987387	-1.486052
38	1	0	5.036111	-1.244461	-1.881625
39	6	0	6.570372	-1.609226	0.488280
40	1	0	6.869246	-1.347661	1.499624
41	1	0	6.941920	-2.599344	0.232910
42	1	0	6.916863	-0.862029	-0.222114
43	16	0	0.114914	-1.611643	-2.962645
44	8	0	1.103851	-1.694543	-1.806340
45	6	0	-1.313163	-2.635496	-2.496628
46	1	0	-1.818822	-2.115775	-1.687966
47	1	0	-1.974741	-2.720688	-3.356407
48	1	0	-0.957995	-3.611725	-2.174171
49	6	0	0.777056	-2.694928	-4.265794
50	1	0	0.052633	-2.752064	-5.075458
51	1	0	1.695073	-2.233725	-4.619746
52	1	0	0.977364	-3.677898	-3.845471
53	16	0	-0.509814	-0.951330	3.713685
54	8	0	-1.376547	-0.844874	2.464467
55	6	0	0.935127	-1.953810	3.249625
56	1	0	1.631554	-1.969451	4.085464
57	1	0	0.569224	-2.957524	3.051154
58	1	0	1.390809	-1.523558	2.361137
59	6	0	0.344222	0.646073	3.878400
60	1	0	-0.416369	1.383028	4.121702
61	1	0	1.066156	0.574070	4.689235
62	1	0	0.825323	0.879908	2.931435

0406qbb_1_8_DAN_HB_+4HOH_TD_b3lyp6311++2d2pdp_PCMw_NOSYMM_optsp.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.988227	-0.107068	0.048706
2	6	0	3.446421	-1.401974	0.056360
3	6	0	2.050209	-1.656652	0.028198
4	6	0	1.135606	-0.559197	-0.008190
5	6	0	1.715675	0.762823	-0.024469
6	6	0	3.133220	0.966836	0.007600
7	1	0	2.274333	-3.812603	0.059365
8	1	0	5.058288	0.037744	0.073197
9	1	0	4.115636	-2.252132	0.084868
10	6	0	1.567616	-2.995303	0.033527
11	6	0	-0.267685	-0.825218	-0.030268
12	1	0	3.500122	1.983531	-0.002277
13	6	0	-0.712318	-2.186786	-0.030264
14	6	0	0.173962	-3.237884	-0.000486
15	1	0	-1.778726	-2.373424	-0.052594
16	1	0	-0.195813	-4.255359	-0.001633
17	7	0	0.927801	1.851194	-0.072733
18	1	0	1.324792	2.786343	-0.094192
19	1	0	-0.082757	1.671358	-0.098167
20	7	0	-1.249099	0.239800	-0.056132
21	1	0	-1.898953	0.116368	-0.829384
22	1	0	-1.822963	0.237585	0.786983
23	8	0	-3.427183	0.463022	2.297393
24	1	0	-4.114221	0.550986	1.606887
25	8	0	-3.843136	0.040967	-2.097153
26	1	0	-3.961069	0.601527	-2.872134
27	8	0	2.155987	4.574482	-0.132320
28	1	0	1.886807	5.163352	0.580679
29	8	0	-5.246697	0.864869	0.202647
30	1	0	-4.832663	0.551956	-0.624667
31	1	0	-3.598141	-0.383396	2.720868
32	1	0	-6.095564	0.415394	0.257222
33	1	0	-4.029909	-0.854458	-2.400555
34	1	0	2.002514	5.074096	-0.941242

0406qcb_1_8_DAN+4HOH_TD_sym_b3lyp6311++2d2p_PCMw_NOSYMM_jo_spopt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.421399	2.374230	0.477161
2	6	0	1.203040	3.053545	0.234151
3	6	0	-0.000040	2.352651	-0.000035
4	6	0	-0.000049	0.906055	0.000008
5	6	0	1.269418	0.260946	0.075155
6	6	0	2.454914	1.009232	0.401064
7	1	0	-1.172950	4.134125	-0.272510
8	1	0	3.316651	2.932932	0.711220
9	1	0	1.172838	4.134160	0.272274
10	6	0	-1.203157	3.053514	-0.234285
11	6	0	-1.269515	0.260954	-0.075085
12	1	0	3.374590	0.462509	0.559630
13	6	0	-2.455046	1.009217	-0.401066
14	6	0	-2.421503	2.374205	-0.477239
15	1	0	-3.374712	0.462475	-0.559599
16	1	0	-3.316749	2.932912	-0.711314
17	7	0	1.451614	-1.111214	-0.119693
18	1	0	2.417375	-1.371246	-0.308299
19	1	0	0.827745	-1.557357	-0.783889
20	7	0	-1.451766	-1.111117	0.119870
21	1	0	-0.827874	-1.557402	0.783941
22	1	0	-2.417547	-1.371225	0.308282
23	8	0	0.526849	-2.513623	2.245522
24	1	0	1.042538	-2.139150	1.502499
25	8	0	-4.331191	-2.020473	0.602314
26	1	0	-4.486498	-2.933242	0.337498

27	8	0	4.331230	-2.020230	-0.602214
28	1	0	4.631729	-1.971143	-1.515814
29	8	0	-0.526543	-2.514013	-2.245557
30	1	0	-1.042819	-2.139831	-1.502854
31	1	0	-4.630832	-1.972449	1.516245
32	1	0	-0.609770	-3.468827	-2.158454
33	1	0	0.610761	-3.468388	2.158532
34	1	0	4.487064	-2.933118	-0.338111

0413caa_1_5_DAN_4DMSO_b3lyp6311++2d2p_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.265255	2.618167	-0.539139
2	6	0	-0.840631	1.805299	-0.627189
3	6	0	-0.684338	0.424542	-0.909739
4	6	0	0.629144	-0.114575	-1.107553
5	6	0	1.766181	0.762027	-0.997602
6	6	0	1.559106	2.105781	-0.718641
7	1	0	0.142749	3.671653	-0.322857
8	1	0	-1.822622	2.226964	-0.476008
9	6	0	-1.820992	-0.453877	-1.011829
10	6	0	0.784344	-1.490309	-1.413410
11	1	0	2.415798	2.762064	-0.638471
12	6	0	-0.321944	-2.301597	-1.510720
13	6	0	-1.614135	-1.794367	-1.308186
14	7	0	3.049156	0.291691	-1.226691
15	1	0	3.797306	0.903077	-0.915086
16	1	0	3.246288	-0.683827	-1.043974
17	1	0	1.766016	-1.910239	-1.569769
18	1	0	-0.200261	-3.351453	-1.744530
19	7	0	-3.109714	0.033575	-0.878201
20	1	0	-3.827853	-0.666696	-0.723899
21	1	0	-3.261193	0.874887	-0.336078
22	1	0	-2.470524	-2.451244	-1.386011
23	16	0	4.705399	-3.481238	0.154435
24	8	0	4.189650	-2.573734	-0.955596
25	16	0	6.277085	1.778775	0.747603
26	8	0	5.335093	2.142116	-0.394778
27	16	0	-5.750435	-2.551247	0.866416
28	8	0	-5.335392	-2.029762	-0.505193
29	16	0	-5.298520	3.176524	-0.010330
30	8	0	-4.096705	2.518560	0.658834
31	6	0	6.319574	3.224176	1.848775
32	1	0	5.333064	3.306055	2.296541
33	1	0	7.067291	3.053475	2.620415
34	1	0	6.551854	4.110031	1.262120
35	6	0	7.961644	1.924596	0.081361
36	1	0	8.671544	1.779281	0.892842
37	1	0	8.074871	1.137554	-0.658997
38	1	0	8.078584	2.904216	-0.376231
39	6	0	6.259610	-2.741451	0.740947
40	1	0	6.605018	-3.299124	1.608886
41	1	0	6.975844	-2.834524	-0.070876
42	1	0	6.087488	-1.695686	0.985289
43	6	0	3.693706	-3.127963	1.623741
44	1	0	2.688178	-3.474801	1.402557
45	1	0	4.102392	-3.680668	2.467003
46	1	0	3.699158	-2.057143	1.812831
47	6	0	-5.014685	-4.205911	1.025238
48	1	0	-3.938769	-4.065720	1.081330
49	1	0	-5.379978	-4.664183	1.941769
50	1	0	-5.281469	-4.798182	0.152965
51	6	0	-7.485920	-3.065386	0.704826
52	1	0	-7.793273	-3.551659	1.628159
53	1	0	-8.067208	-2.161068	0.547674
54	1	0	-7.579079	-3.736621	-0.145796
55	6	0	-6.575578	3.326447	1.274435
56	1	0	-7.413087	3.890647	0.869664
57	1	0	-6.890817	2.316425	1.521244
58	1	0	-6.148825	3.820724	2.144076
59	6	0	-4.890182	4.941340	-0.162585

60	1	0	-4.080132	5.013904	-0.882998
61	1	0	-5.765406	5.472504	-0.530561
62	1	0	-4.577640	5.318420	0.808528

0413cca_1_5_DAN_4DMSO_TD_b3lyp6311++2d2p_PCMdmso_opt.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.327577	2.505808	0.127885
2	6	0	-0.820205	1.687362	-0.036744
3	6	0	-0.698134	0.293300	-0.219440
4	6	0	0.625851	-0.292017	-0.272158
5	6	0	1.761198	0.560814	-0.138517
6	6	0	1.585953	1.970194	0.085264
7	1	0	0.198135	3.568543	0.285053
8	1	0	-1.793826	2.153298	0.003929
9	6	0	-1.832402	-0.562270	-0.358824
10	6	0	0.745902	-1.686868	-0.450690
11	1	0	2.464954	2.588476	0.205698
12	6	0	-0.398808	-2.508649	-0.613626
13	6	0	-1.657081	-1.973556	-0.575084
14	7	0	3.044943	0.076657	-0.146089
15	1	0	3.804166	0.749461	-0.207228
16	1	0	3.261020	-0.846835	-0.503413
17	1	0	1.720402	-2.150965	-0.491890
18	1	0	-0.267256	-3.571332	-0.768245
19	7	0	-3.111790	-0.084774	-0.341725
20	1	0	-3.884785	-0.744705	-0.350891
21	1	0	-3.338169	0.864952	-0.069561
22	1	0	-2.535910	-2.591287	-0.698378
23	16	0	5.146257	-3.502294	-0.597133
24	8	0	4.114123	-2.569185	-1.223306
25	16	0	6.446043	2.010530	0.643055
26	8	0	5.286208	2.064665	-0.347079
27	16	0	-5.992250	-2.571186	0.805538
28	8	0	-5.446879	-1.927859	-0.466843
29	16	0	-5.338818	3.114436	-0.475891
30	8	0	-4.202968	2.623962	0.417997
31	6	0	6.373584	3.556947	1.594862
32	1	0	5.473219	3.509862	2.201199
33	1	0	7.252094	3.613232	2.234061
34	1	0	6.331294	4.396896	0.905321
35	6	0	7.943941	2.378983	-0.317456
36	1	0	8.784208	2.466887	0.367894
37	1	0	8.098038	1.541282	-0.991874
38	1	0	7.790140	3.299986	-0.874909
39	6	0	6.440317	-2.437780	0.108515
40	1	0	7.137056	-3.060461	0.665450
41	1	0	6.948379	-1.965408	-0.727659
42	1	0	5.977356	-1.691832	0.750621
43	6	0	4.428397	-4.087385	0.967431
44	1	0	3.584596	-4.720874	0.708200
45	1	0	5.180532	-4.666086	1.499314
46	1	0	4.101381	-3.230138	1.551942
47	6	0	-6.055280	-4.357274	0.478182
48	1	0	-5.026472	-4.697137	0.398307
49	1	0	-6.546983	-4.848510	1.315101
50	1	0	-6.591811	-4.528257	-0.452200
51	6	0	-7.781088	-2.252036	0.802356
52	1	0	-8.232293	-2.788327	1.634419
53	1	0	-7.908227	-1.181329	0.935567
54	1	0	-8.197382	-2.574919	-0.149036
55	6	0	-6.523674	3.937300	0.629257
56	1	0	-7.299787	4.402670	0.025456
57	1	0	-6.954158	3.162806	1.257942
58	1	0	-5.995123	4.673251	1.230767
59	6	0	-4.712605	4.595973	-1.322087
60	1	0	-3.927183	4.262204	-1.994668
61	1	0	-5.525242	5.043775	-1.890114
62	1	0	-4.318681	5.288102	-0.581502

0413q_aac_1_5_DAN_4HOH_b3lyp6311++2d2p_PCMw_sp_assym.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.467305	2.480901	-0.323046
2	6	0	-0.692044	1.741974	-0.313653
3	6	0	-0.632044	0.325567	-0.296214
4	6	0	0.642828	-0.328623	-0.302137
5	6	0	1.836589	0.474459	-0.293333
6	6	0	1.724047	1.856594	-0.305489
7	1	0	0.417160	3.561781	-0.338865
8	1	0	-1.644119	2.249772	-0.327188
9	6	0	-1.825852	-0.477313	-0.283330
10	6	0	0.703119	-1.744967	-0.326886
11	1	0	2.624087	2.457487	-0.301423
12	6	0	-0.456597	-2.483522	-0.331079
13	6	0	-1.713184	-1.859397	-0.302063
14	7	0	3.088758	-0.122939	-0.335325
15	1	0	3.862452	0.488747	-0.104963
16	1	0	3.189867	-1.036412	0.085823
17	1	0	1.654834	-2.252905	-0.350023
18	1	0	-0.406695	-3.564328	-0.352198
19	7	0	-3.078213	0.119695	-0.315579
20	1	0	-3.851634	-0.492321	-0.085274
21	1	0	-3.179200	1.032767	0.105729
22	1	0	-2.613121	-2.460425	-0.294504
23	8	0	3.939853	-2.920520	0.836846
24	1	0	4.901724	-2.945783	0.874734
25	8	0	5.531103	1.726093	0.293633
26	1	0	5.842388	1.702382	1.204504
27	8	0	-5.532183	-1.719524	0.298262
28	1	0	-6.243854	-1.585085	-0.336341
29	8	0	-4.072987	2.830182	0.915729
30	1	0	-3.556824	3.319251	1.564954
31	1	0	-4.343137	3.489631	0.268146
32	1	0	-5.939452	-1.578567	1.159362
33	1	0	3.651762	-3.135118	1.730189
34	1	0	6.308653	1.527949	-0.238709

0413qdab_1_5_DAN_5HOH_TD_b3lyp6311++2d2p_PCMw_spopt_assym.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.704492	-2.474368	0.056517
2	6	0	-0.456401	-1.663877	0.051704
3	6	0	-0.387803	-0.252314	-0.011742
4	6	0	0.910109	0.376599	-0.022762
5	6	0	2.067133	-0.465586	-0.008980
6	6	0	1.943866	-1.898200	0.022510
7	1	0	0.602247	-3.549888	0.089219
8	1	0	-1.418765	-2.152382	0.094398
9	6	0	-1.551013	0.563081	-0.054567
10	6	0	0.995019	1.786060	-0.040708
11	1	0	2.845395	-2.494502	0.022939
12	6	0	-0.188257	2.573358	-0.025063
13	6	0	-1.427612	1.986651	-0.027767
14	7	0	3.322774	0.044463	-0.033686
15	1	0	4.121731	-0.581065	-0.024583
16	1	0	3.520494	1.036142	-0.068568
17	1	0	1.950901	2.286764	-0.035727
18	1	0	-0.103731	3.652027	-0.018080
19	7	0	-2.840409	-0.000398	-0.009785
20	1	0	-3.568828	0.656590	-0.276086
21	1	0	-2.962275	-0.865531	-0.528924
22	1	0	-2.325682	2.589945	-0.024418
23	8	0	4.448734	2.870972	-0.132338
24	1	0	5.085279	3.010684	0.576611
25	8	0	5.674490	-1.831249	-0.014227
26	1	0	6.212340	-1.804430	-0.812635

27	8	0	-5.185767	1.933159	-0.717990
28	1	0	-6.008142	1.664382	-0.295127
29	8	0	-3.750429	-2.563046	-1.561118
30	1	0	-3.125481	-2.986062	-2.159403
31	1	0	4.940734	3.030019	-0.944668
32	1	0	6.296414	-1.707440	0.710600
33	1	0	-4.076903	-3.275609	-1.001532
34	1	0	-5.394975	1.981359	-1.656673
35	8	0	-3.608685	-0.690100	2.700899
36	1	0	-3.331694	-0.475415	1.780843
37	1	0	-2.919558	-1.270356	3.039461
