Supporting Information

for

Optical Investigation of 2-amino-7-isocyanofluorene, a Novel Blue-Emitting Solvatochromic Dye

Bence Kontra [1,2], Zoltán Mucsi [2,3], László Vanyorek [3] and Miklós Nagy [3,*]

[1] Department of Organic Chemistry, Semmelweis University, Hőgyes Endre utca 7, H-1092 Budapest, Hungary; bence.kontra@femtonics.eu

[2] Brain Vision Center, Department of Chemistry, Vendel utca 9, H-1094 Budapest, Hungary; zoltanmucsi@gmail.com

[3] Institute of Chemistry, University of Miskolc, Miskolc-Egyetemváros, H-3515 Miskolc, Hungary; kemvanyi@uni-miskolc.hu

* Correspondence: nagy.miklos@uni-miskolc.hu

Table of Contents

Figure S1. ¹H-NMR spectrum of 2-amino-7-isocyanofluorene (**2,7-ICAF**) recorded at 400 MHz in DMSO-*d₆*.

Figure S2. ^{13}C NMR spectrum of 2-amino-7-isocyanofluorene (**2,7-ICAF**) recorded at 101 MHz in DMSO-d_6.
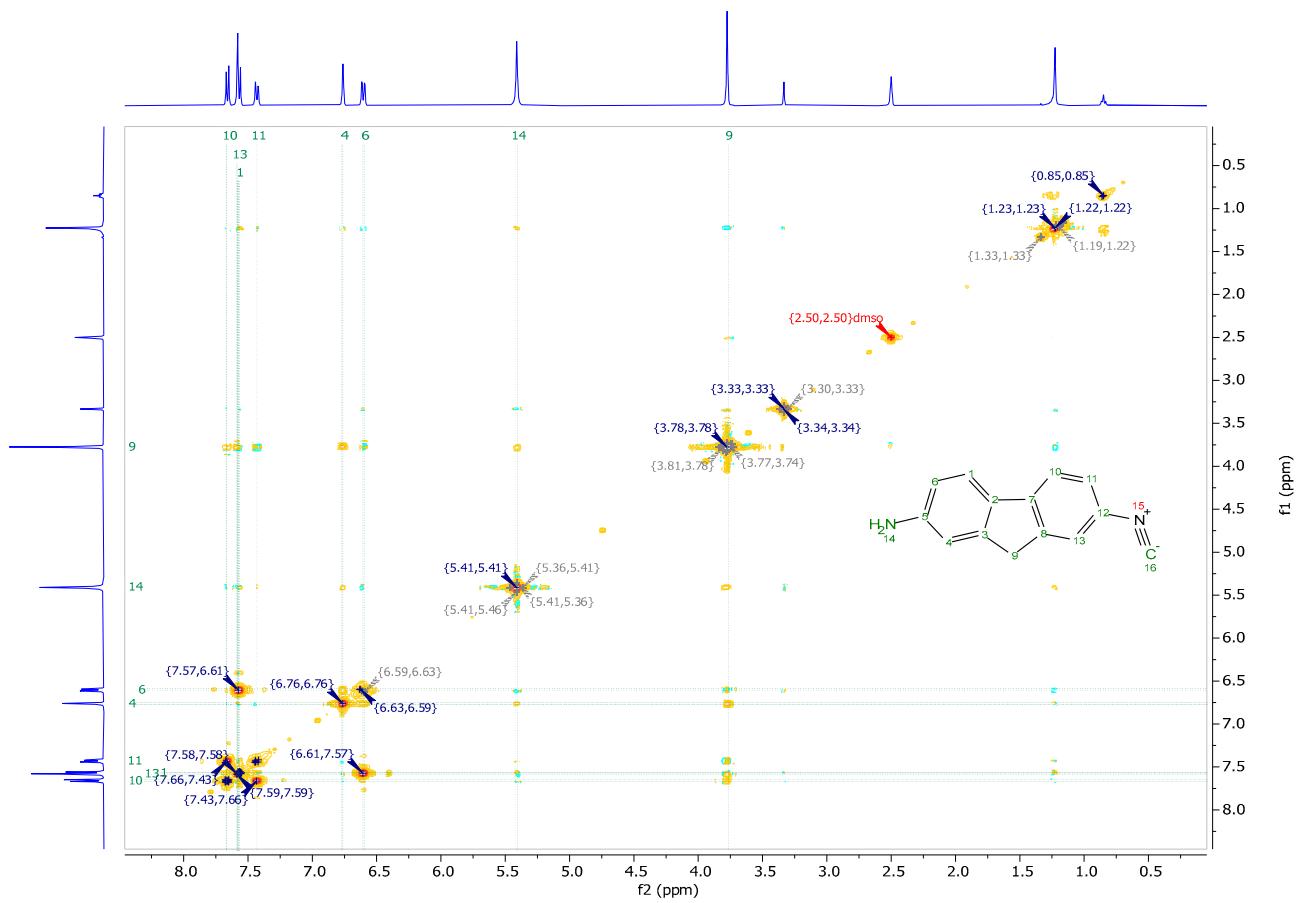
Figure S3. COSY spectrum of 2-amino-7-isocyanofluorene (**2,7-ICAF**) recorded at 400 MHz in DMSO-*d₆*.
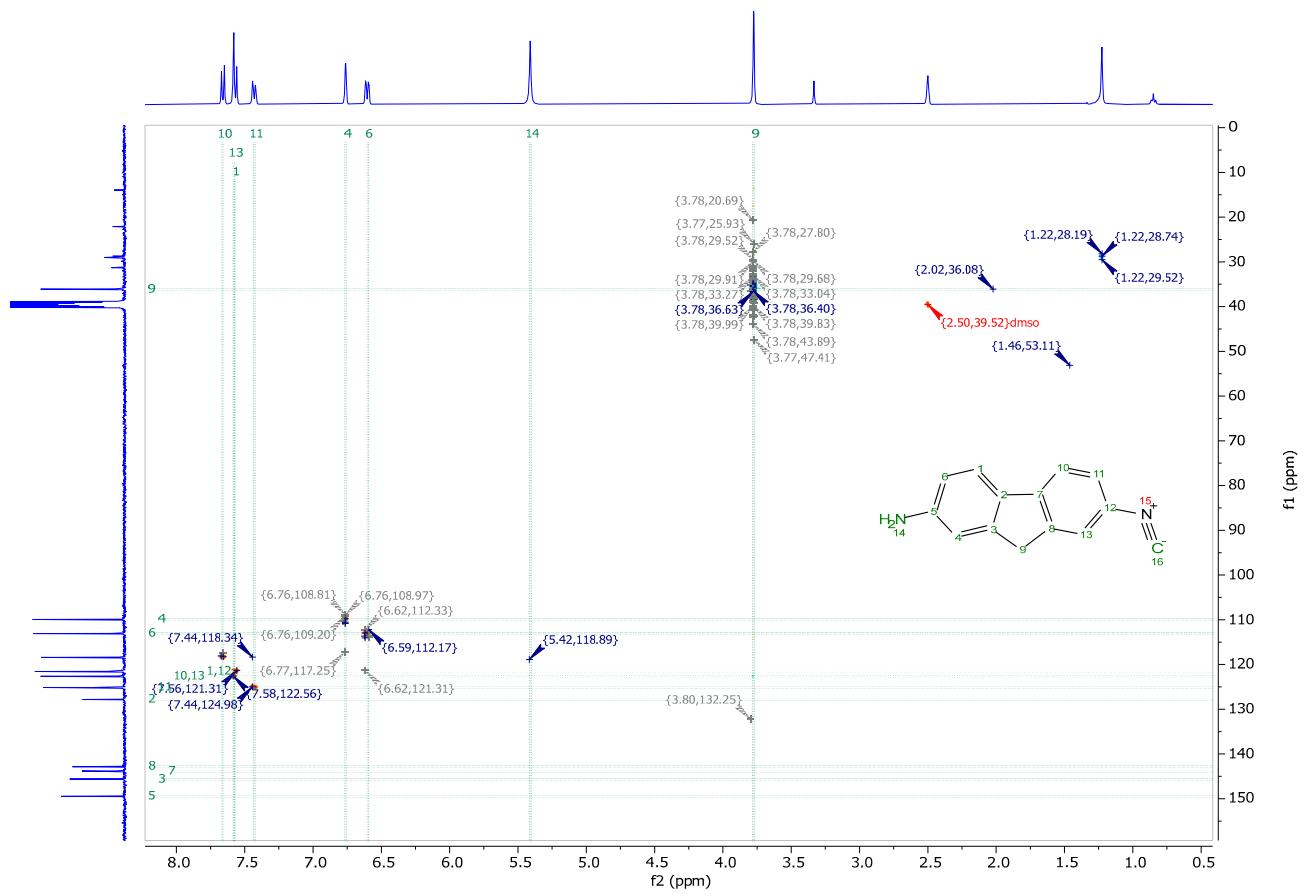
Figure S4. HSQC spectrum of 2-amino-7-isocyanofluorene (**2,7-ICAF**) recorded at 400 MHz and 101 MHz in DMSO-*d₆*.
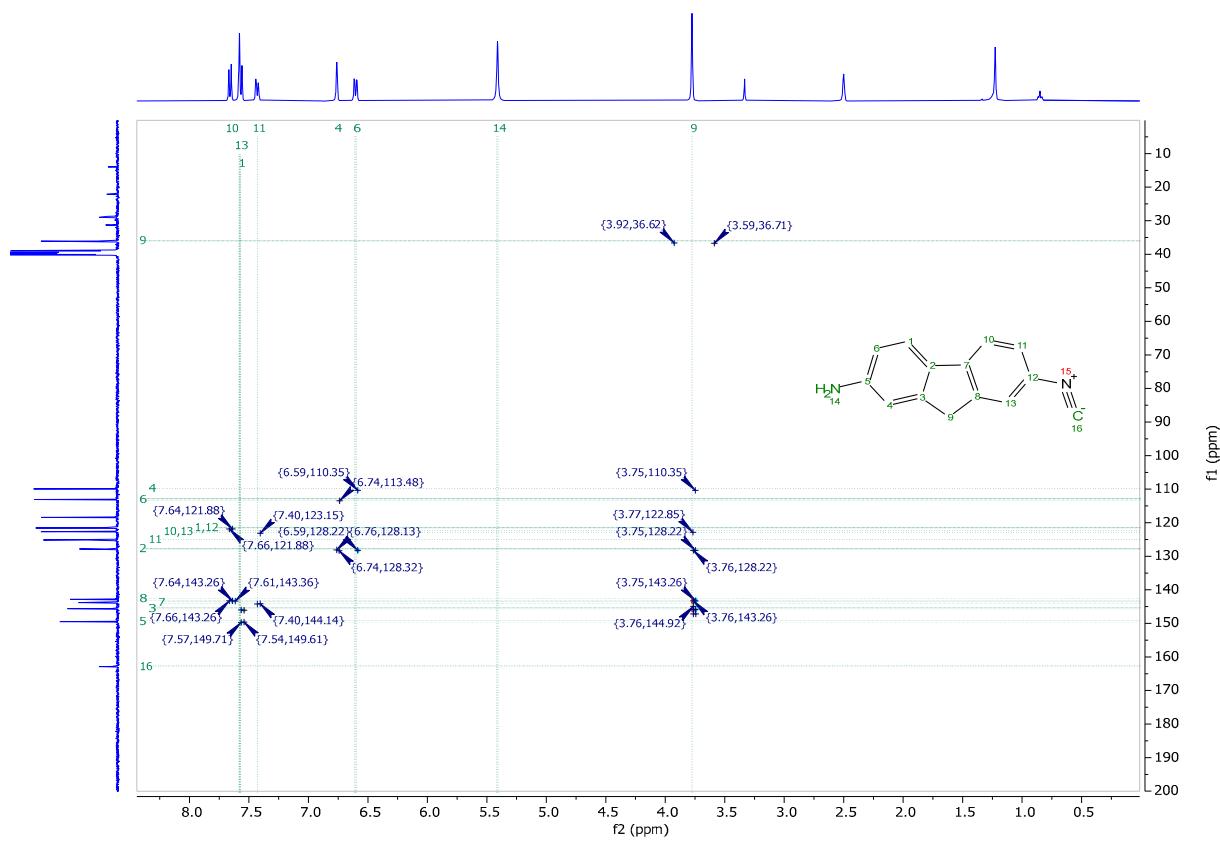
Figure S5. HMBC spectrum of 2-amino-7-isocyanofluorene (**2,7-ICAF**) recorded at 400 MHz and 101 MHz in DMSO-*d₆*.
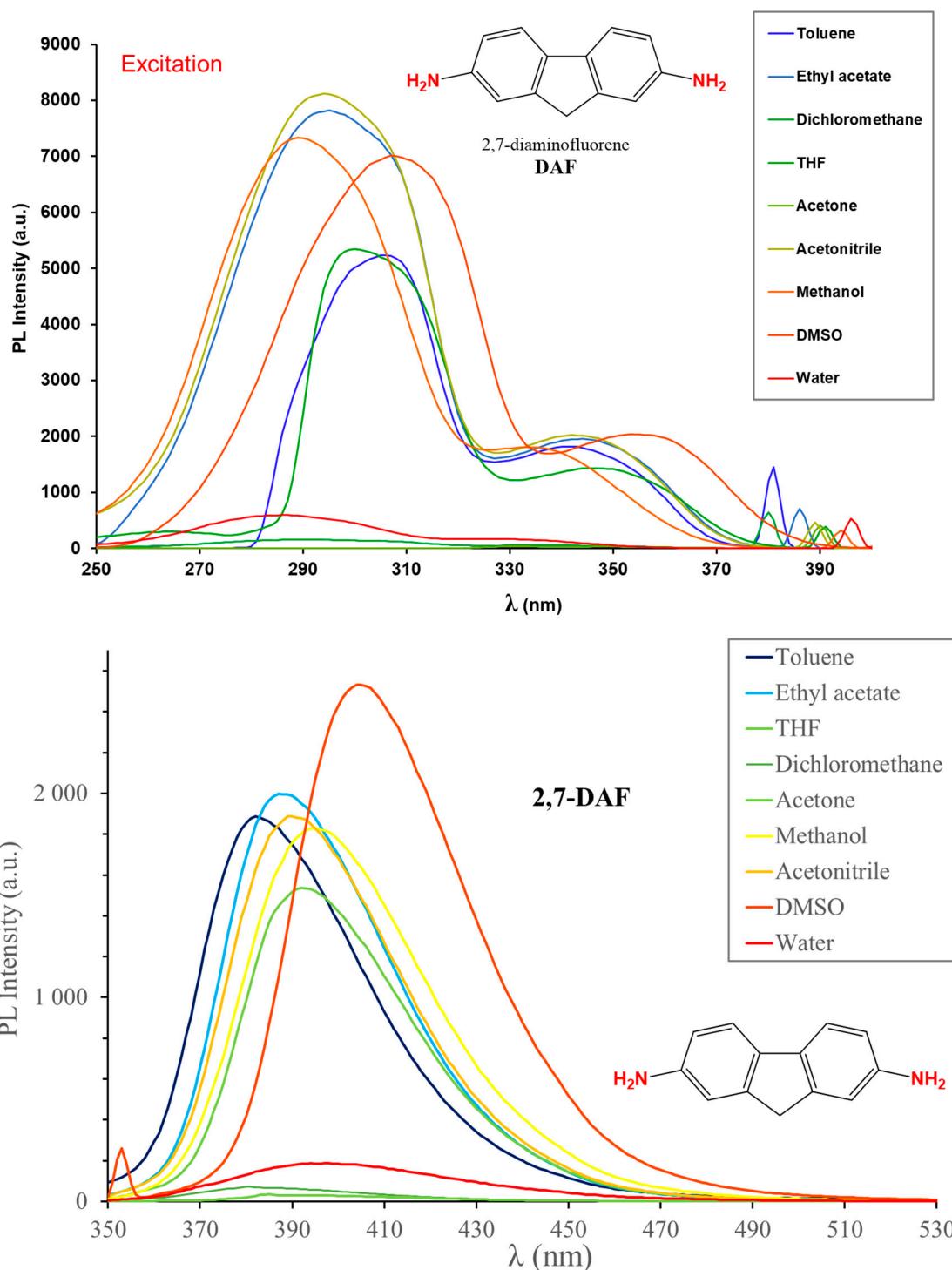
Figure S6. Steady-state fluorescence (**top**) excitation, (**bottom**) emission spectra of 2,7-DAF recorded in various solvents of different polarity. ([dye] = 7.40 × 10^{-6} M, T=20 ºC).
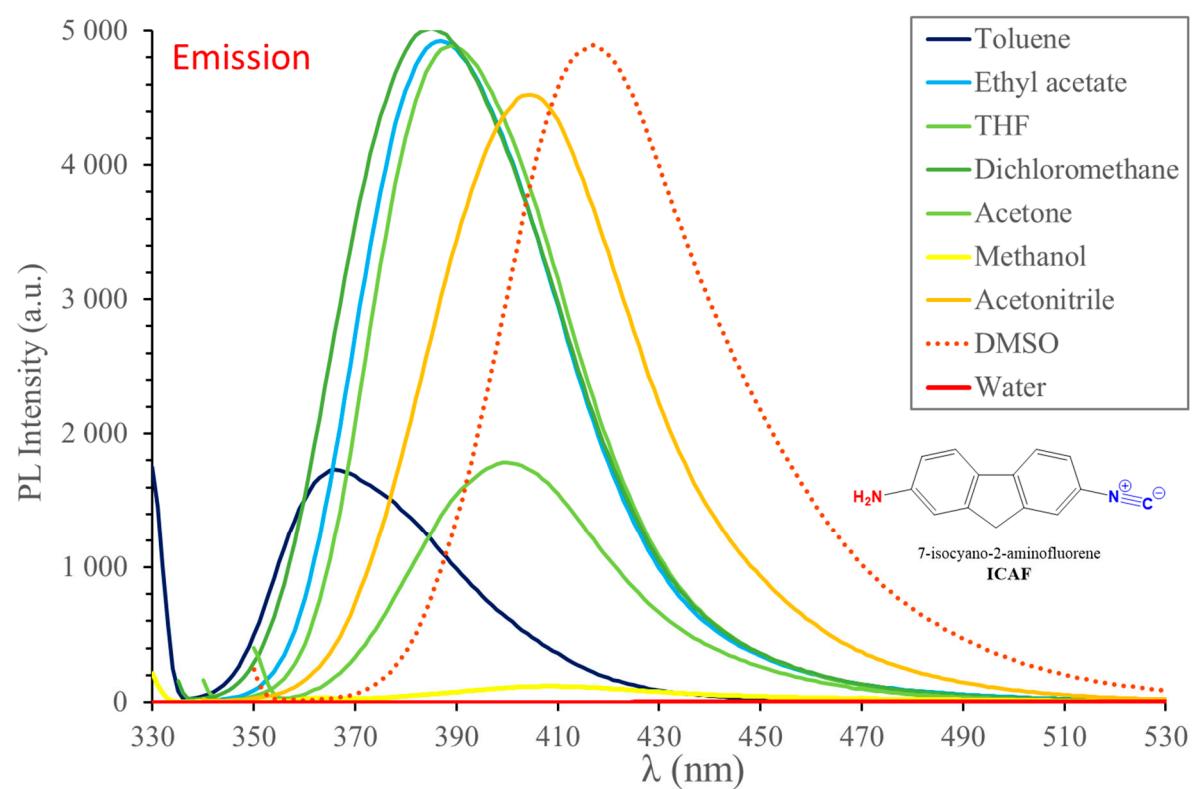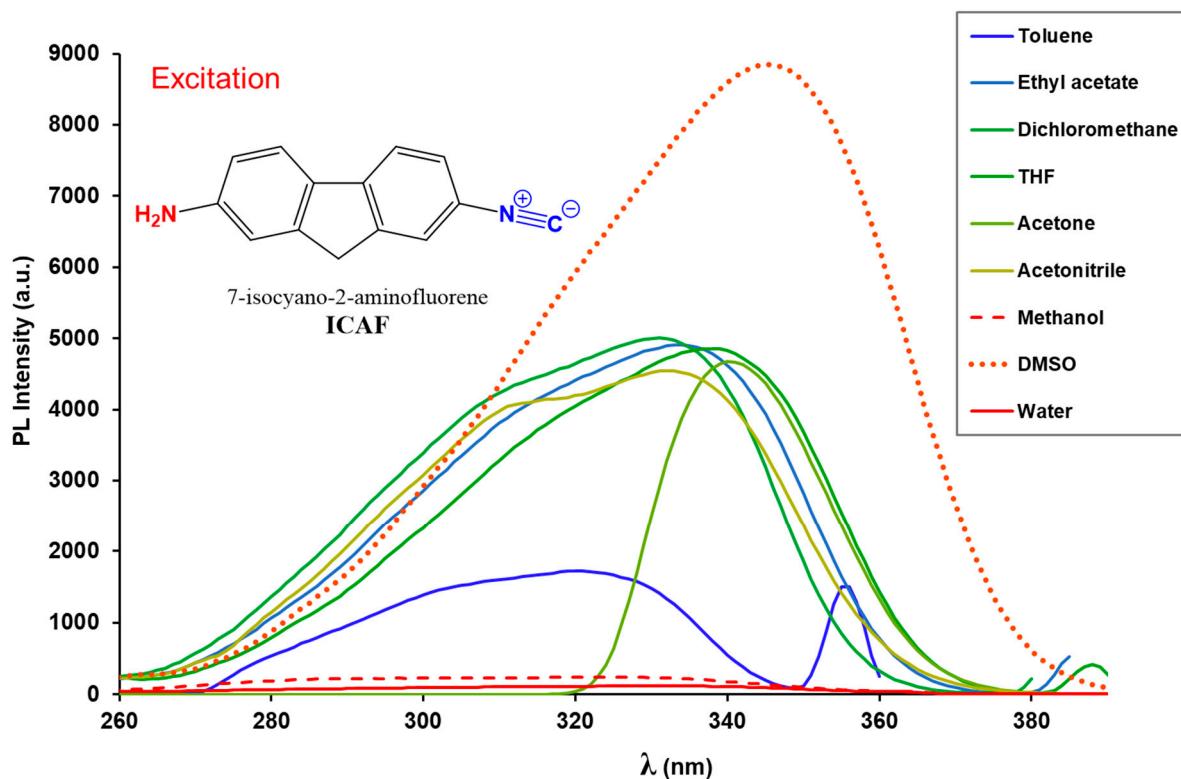
Figure S7. Steady-state fluorescence (**top**) excitation, (**bottom**) emission spectra of **2,7-ICAF** recorded in various solvents of different polarity. ([dye] = 4.84 × 10⁻⁶ M, T=20 ºC).
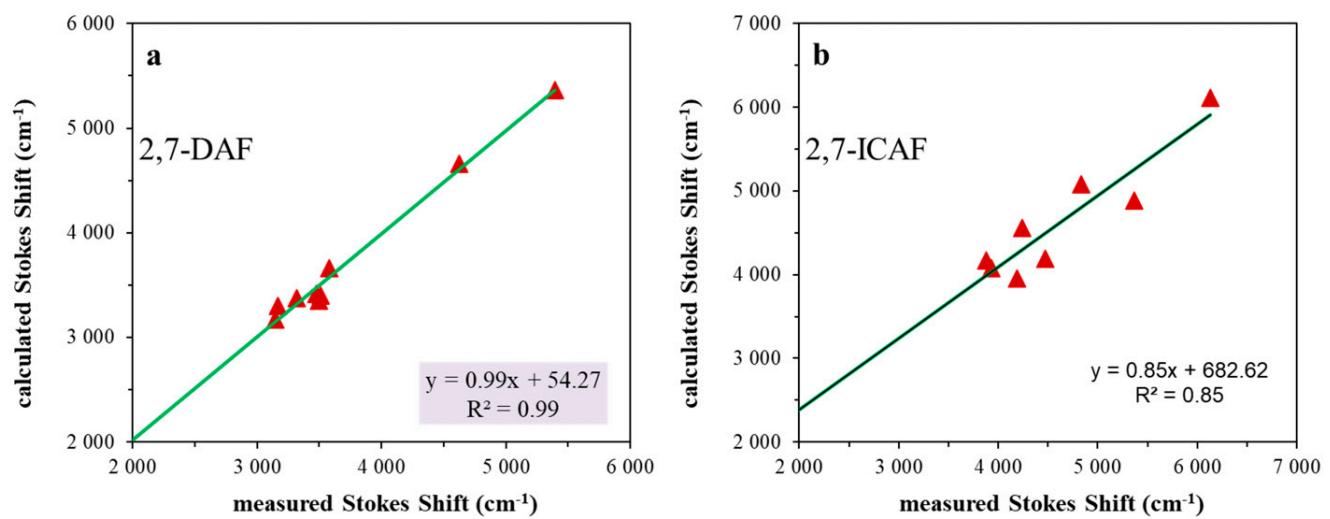
Figure S8. Catalán plots for the (**a**) 2,7-diamino-fluorene (**2,7-DAF**) and (**b**) 2-amino-7-isocyano-fluorene (**2,7-ICAF**).
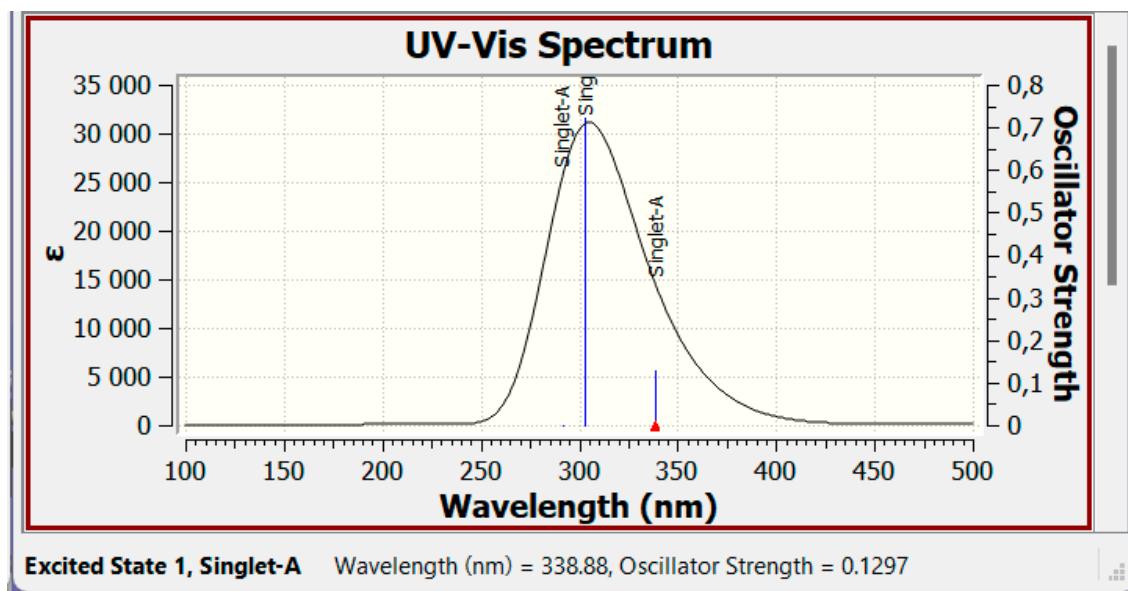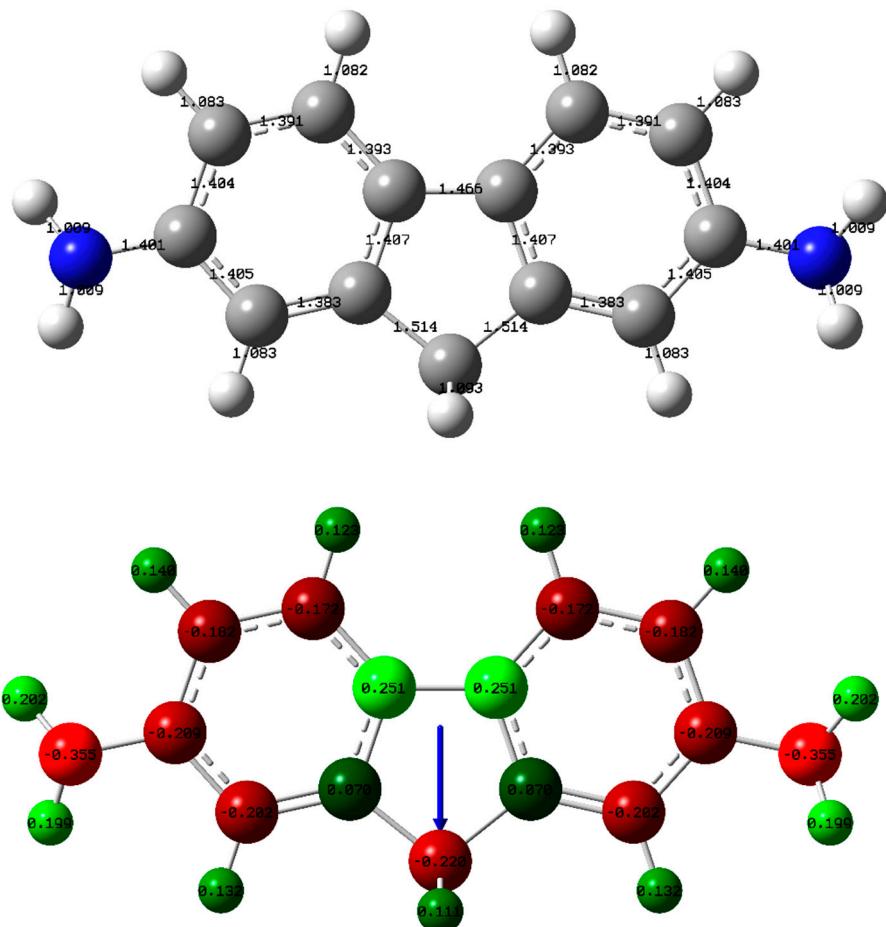
Figure S9. The optimized geometry of 2,7-DAF in the ground S_0 state calculated on the TD-B3LYP/6-311++G(2d,2p)//PCM(solvent level of theory. Bond lengths (top), Charge distribution and dipole moment (middle), Vertical excitation (bottom).
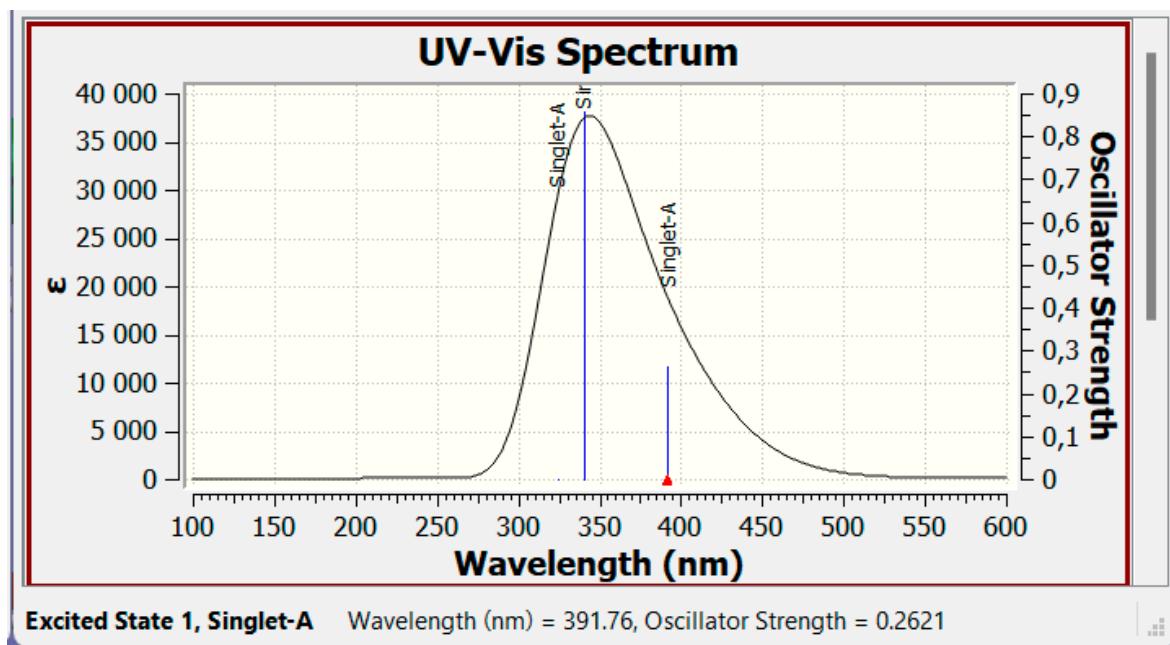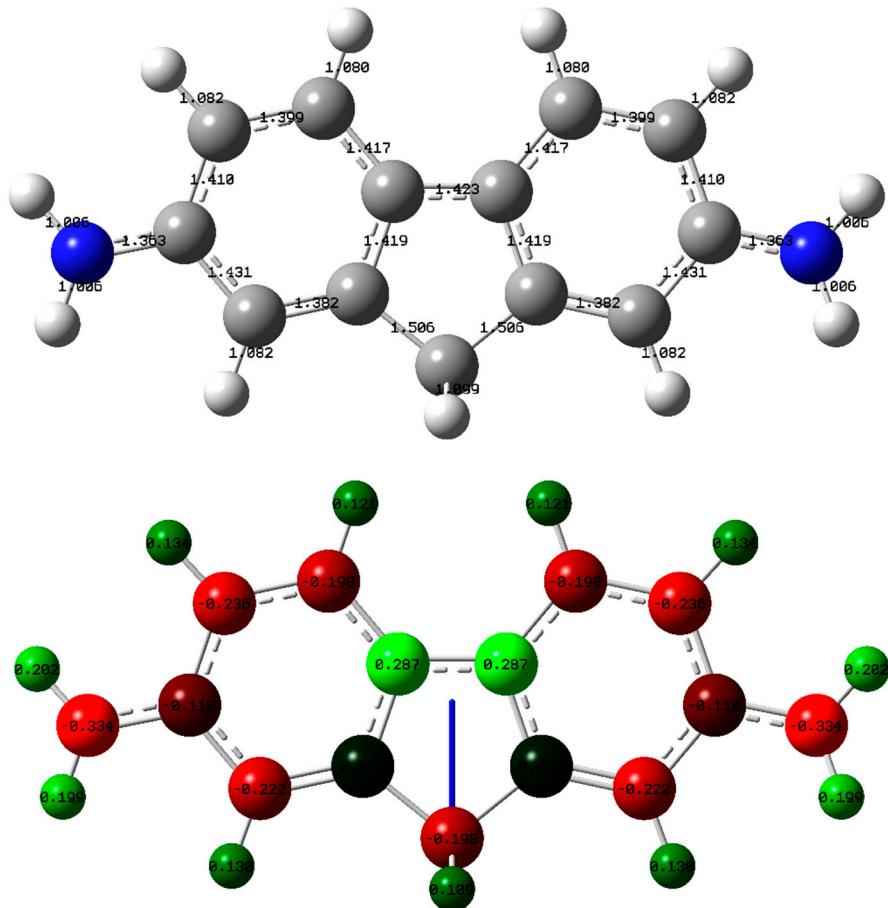
Figure S10. The optimized geometry of 2,7-DAF in the first excited S_1 state calculated on the TD-B3LYP/6-311++G(2d,2p)//PCM(solvent level of theory. Bond lengths (top), Charge distribution and dipole moment (middle), Emission spectrum (bottom).
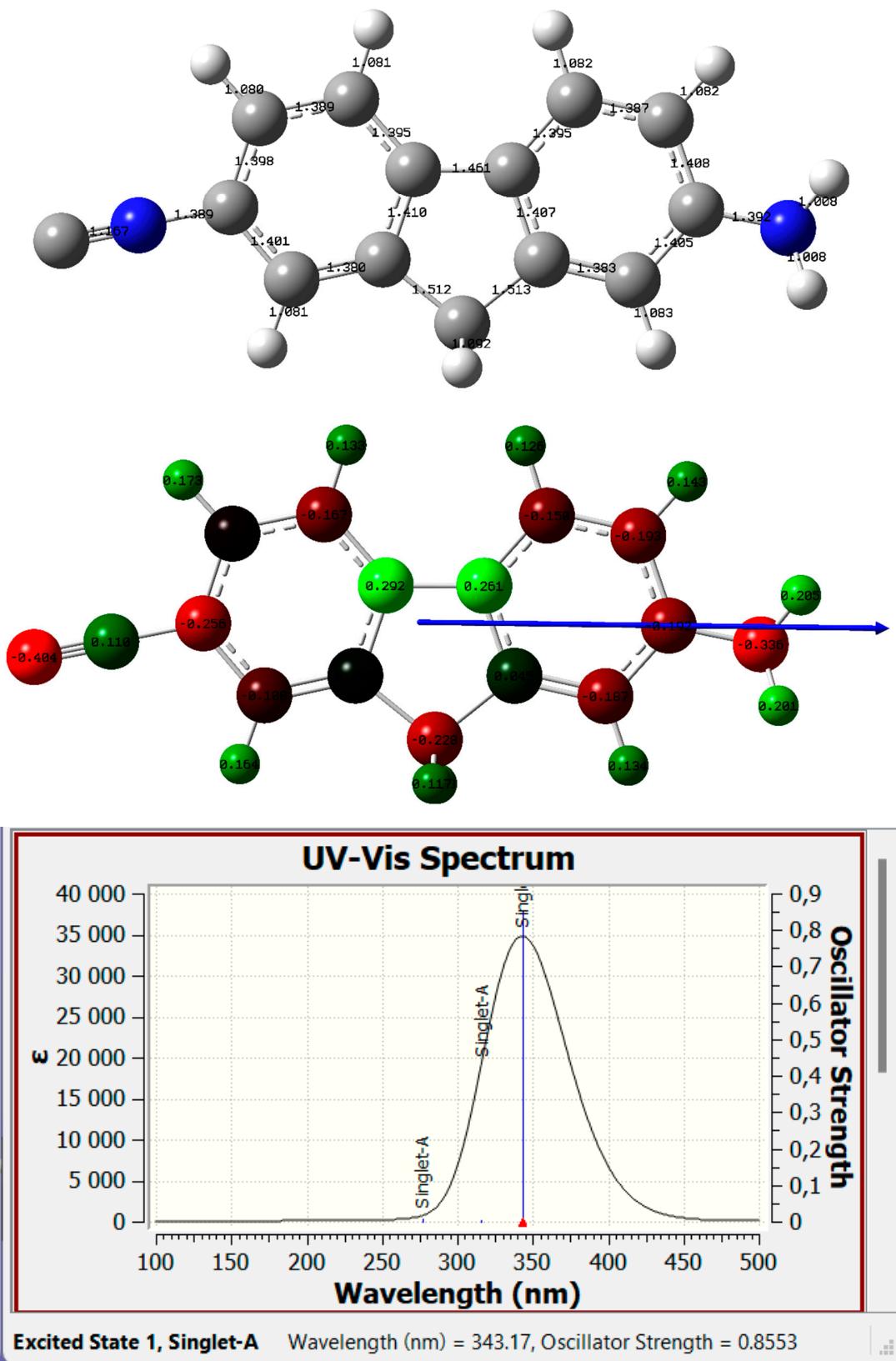
Figure S11. The optimized geometry of 2,7-ICAF in the ground S$_0$ state calculated on the TD-B3LYP/6-311++G(2d,2p)//PCM(solvent level of theory. Bond lengths (top), Charge distribution and dipole moment (middle), Vertical excitation (bottom).
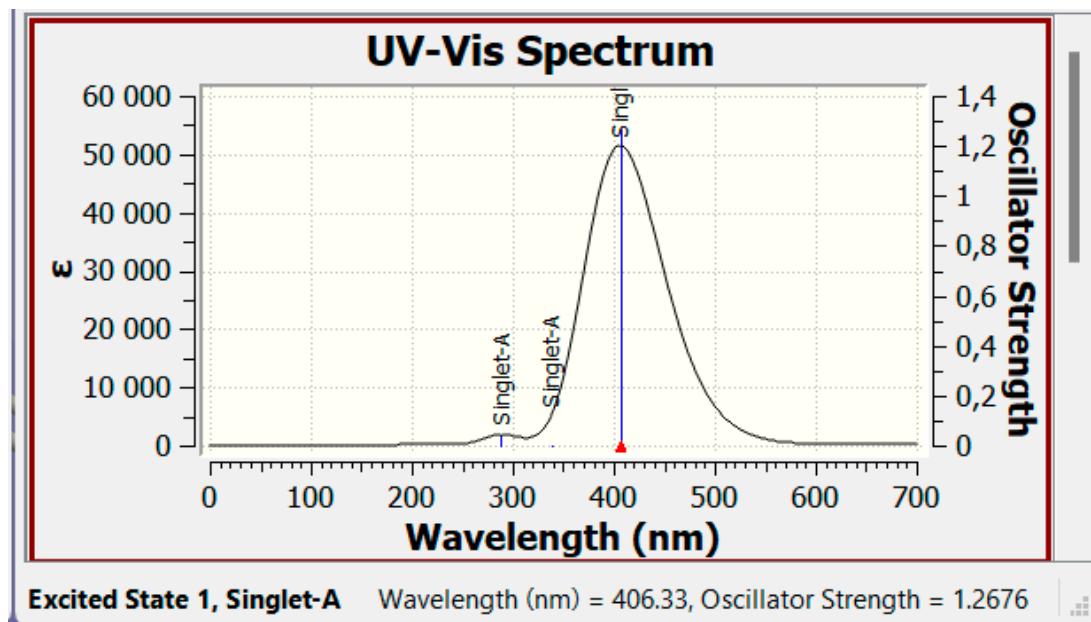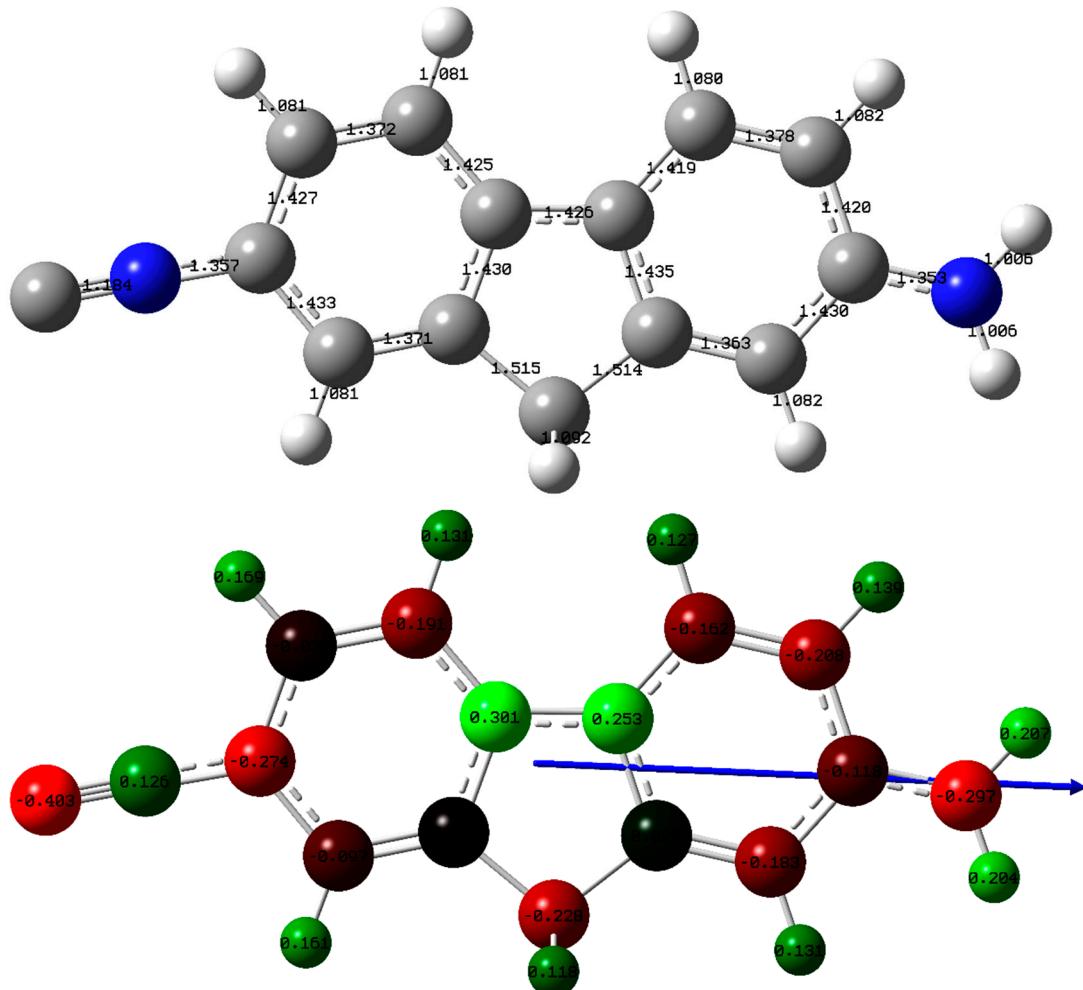
Figure S12. The optimized geometry of 2,7-ICAF in the first excited S_1 state calculated on the TD-B3LYP/6-311++G(2d,2p)//PCM(solvent level of theory. Bond lengths (top), Charge distribution and dipole moment (middle), Emission spectrum (bottom).

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 (DMSO). 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(DMSO)[4] level of theory using the geometries optimized at B3LYP/6-311++G(2d,2p)//PCM(DMSO). The emission wavelengths were calculated after optimization using geometries provided by TD-B3LYP/6-311++G(2d,2p)//PCM(DMSO).

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.

Raw computational data

Table S1. 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 DMSO for ground (S0), single point excited (S$_1$) as well as excited (S$_1$*) state of 2,7-DAF; 2,7-ICAF; DAB and ICAB.

Comp.	State	Filenev			E	ZPE	U	H	G	S
2,7-DAF	S$_0$	0501aaa_mol1_B3LYP6311++2d2p_PCMdmso.log			-612.33098784	-612.110599	-612.098633	-612.097689	-612.147918	105.717
	S$_1$	0501aab_mol1_TD_B3LYP6311++2d2p_PCMdmso_sp.log	339	0.130	-612.19653000	–	–	–	–	–
			303	0.723						
	S$_1$*	0501aac_mol1_TD_B3LYP6311++2d2p_PCMdmso_opt.log	392	0.262	-612.20649000	–	–	–	–	–
			340	0.860						
2,7-ICAF	S$_0$	0503aaa_mol1_CN_B3LYP6311++2d2p_PCMdmso.log			-649.18940909	-648.987660	-648.975234	-648.974290	-649.026067	108.973
	S$_1$	0503aab_mol1_CN_TD_B3LYP6311++2d2p_PCMdmso_sp.log	343	0.855	-649.05664000	–	–	–	–	–
	S$_1$*	0503aac_mol1_CN_TD_B3LYP6311++2d2p_PCMdmso_opt.log	406	1.267	-649.07056000					
DAB	S$_0$	0801aaa_H2NPhPhNH2_b3lyp6311++2d2p_PCMdmso.log			-574.20925824	-573.995095	-573.983253	-573.982309	-574.032946	106.573
	S$_1$	0801baa_H2NPhPhNH2_TD_b3lyp6311++2d2p_PCMdmso_sp.log	298	0.819	-574.06003000	–	–	–	–	–
	S$_1$*	0801caa_H2NPhPhNH2_TD_b3lyp6311++2d2p_PCMdmso_opt.log	388	1.196	-574.07932000					
ICAB	S$_0$	0831aaa_CNPhPhNH2_b3lyp6311++2d2p_PCMdmso.log			-611.06585651	-610.870370	-610.858041	-610.857096	-610.909329	109.933
	S$_1$	0831baa_CNPhPhNH2_TD_b3lyp6311++2d2p_PCMdmso_sp.log	339	0.732	-610.93145000	–	–	–	–	–
	S$_1$*	0831caa_CNPhPhNH2_TD_b3lyp6311++2d2p_PCMdmso_opt.log	413	1.312	-610.94726000					

The xyz coordinates of computed geometries

0501aaa_mol1_B3LYP6311++2d2p_PCMdmso.log

Standard orientation:
```
---------------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number    Type       X        Y         Z
---------------------------------------------------------------------
  1       1        0      0.002980  -2.401882   0.874888
  2       6        0      3.024060   1.267556  -0.003493
  3       6        0      3.475956  -0.061448  -0.007374
  4       6        0      2.533963  -1.103356  -0.007366
  5       6        0      1.183595  -0.802722  -0.004454
  6       6        0      0.732906   0.530293  -0.002534
  7       6        0      1.665219   1.565736  -0.000909
  8       1        0      3.750045   2.070667  -0.002616
  9       1        0      2.873299  -2.132261  -0.010436
 10       1        0      1.348298   2.600536   0.004741
 11       6        0      0.000001  -1.747548  -0.000312
 12       1        0     -0.002973  -2.401385  -0.875975
 13       6        0     -1.183583  -0.802712   0.003637
 14       6        0     -2.533972  -1.103361   0.007132
 15       6        0     -3.475947  -0.061475   0.007888
 16       6        0     -3.024050   1.267557   0.003770
 17       6        0     -1.665234   1.565744   0.000485
 18       6        0     -0.732905   0.530281   0.001670
 19       1        0     -2.873271  -2.132277   0.010139
 20       1        0     -3.750073   2.070627   0.003407
 21       1        0     -1.348303   2.600539  -0.005828
 22       7        0     -4.846484  -0.344309   0.078817
 23       1        0     -5.443851   0.383078  -0.284269
 24       7        0      4.846516  -0.344393  -0.077453
 25       1        0      5.443758   0.383267   0.285287
 26       1        0     -5.109831  -1.243753  -0.294728
 27       1        0      5.109634  -1.243520   0.297006
---------------------------------------------------------------------
```

0501aab_mol1_TD_B3LYP6311++2d2p_PCMdmso_sp.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.002980	-2.401882	-0.874888
2	6	0	-3.024060	1.267556	0.003493
3	6	0	-3.475956	-0.061448	0.007374
4	6	0	-2.533963	-1.103356	0.007366
5	6	0	-1.183595	-0.802722	0.004454
6	6	0	-0.732906	0.530293	0.002534
7	6	0	-1.665219	1.565736	0.000909
8	1	0	-3.750045	2.070667	0.002616
9	1	0	-2.873299	-2.132261	0.010436
10	1	0	-1.348298	2.600536	-0.004741
11	6	0	-0.000001	-1.747548	0.000312
12	1	0	0.002973	-2.401385	0.875975
13	6	0	1.183583	-0.802712	-0.003637
14	6	0	2.533972	-1.103361	-0.007132
15	6	0	3.475947	-0.061475	-0.007888
16	6	0	3.024050	1.267557	-0.003770
17	6	0	1.665234	1.565744	-0.000485
18	6	0	0.732905	0.530281	-0.001670
19	1	0	2.873271	-2.132277	-0.010139
20	1	0	3.750073	2.070627	-0.003407
21	1	0	1.348303	2.600539	0.005828
22	7	0	4.846484	-0.344309	-0.078817
23	1	0	5.443851	0.383078	0.284269
24	7	0	-4.846516	-0.344393	0.077453
25	1	0	-5.443758	0.383267	-0.285287
26	1	0	5.109831	-1.243753	0.294728
27	1	0	-5.109634	-1.243520	-0.297006

0501aac_mol1_TD_B3LYP6311++2d2p_PCMdmso_opt.log

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	-0.000720	-2.450979	-0.875539
2	6	0	-2.989642	1.295215	0.001643
3	6	0	-3.446140	-0.039368	0.001974
4	6	0	-2.523686	-1.133269	0.002577
5	6	0	-1.172343	-0.841526	0.000963
6	6	0	-0.711276	0.500261	0.000593
7	6	0	-1.621087	1.586537	0.001614
8	1	0	-3.721301	2.092655	0.002311
9	1	0	-2.893799	-2.149521	0.005445
10	1	0	-1.270140	2.608149	-0.000449
11	6	0	0.000000	-1.786174	0.000001
12	1	0	0.000720	-2.450975	0.875544
13	6	0	1.172343	-0.841526	-0.000963
14	6	0	2.523687	-1.133269	-0.002577
15	6	0	3.446140	-0.039368	-0.001974
16	6	0	2.989642	1.295215	-0.001643
17	6	0	1.621087	1.586537	-0.001613
18	6	0	0.711276	0.500261	-0.000594
19	1	0	2.893800	-2.149521	-0.005452
20	1	0	3.721301	2.092655	-0.002308
21	1	0	1.270140	2.608149	0.000444
22	7	0	4.782920	-0.306020	-0.034329
23	1	0	5.447341	0.434462	0.112210
24	7	0	-4.782920	-0.306020	0.034329
25	1	0	-5.447341	0.434463	-0.112209
26	1	0	5.110958	-1.241206	0.136096
27	1	0	-5.110958	-1.241206	-0.136099

0503aaa_mol1_CN_B3LYP6311++2d2p_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.190432	-2.393445	0.874981
2	6	0	2.760531	1.348837	-0.000738
3	6	0	3.211768	0.025936	-0.001208
4	6	0	2.316980	-1.051610	-0.001381
5	6	0	0.963942	-0.778072	-0.000813
6	6	0	0.493947	0.551791	-0.000339
7	6	0	1.397617	1.614983	-0.000358
8	1	0	3.480627	2.153672	-0.000429
9	1	0	2.694876	-2.064066	-0.001695
10	1	0	1.054438	2.640087	0.000307
11	6	0	-0.202968	-1.739597	-0.000037
12	1	0	-0.192781	-2.391588	-0.876552
13	6	0	-1.397209	-0.811199	0.002425
14	6	0	-2.742478	-1.129948	0.004240
15	6	0	-3.696157	-0.098127	0.005024
16	6	0	-3.261063	1.240724	0.001011
17	6	0	-1.910386	1.555523	-0.001223
18	6	0	-0.966646	0.528323	0.001094
19	1	0	-3.069401	-2.162304	0.006016
20	1	0	-3.998508	2.032768	0.000265
21	1	0	-1.605245	2.593424	-0.006717
22	7	0	-5.054875	-0.392874	0.072206
23	1	0	-5.673369	0.327595	-0.266162
24	7	0	4.578056	-0.226208	-0.001253
25	1	0	-5.320453	-1.304708	-0.265833
26	6	0	5.725118	-0.440540	-0.001170

0503aab_mol1_CN_TD_B3LYP6311++2d2p_PCMdmso_sp.log

Standard orientation:

Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type   X   Y   Z
----
  1   1   0   0.190432   -2.393445   -0.874981
  2   6   0   -2.760531   1.348837   0.000738
  3   6   0   -3.211768   0.025936   0.001208
  4   6   0   -2.316980   -1.051610   0.001381
  5   6   0   -0.963942   -0.778072   0.000813
  6   6   0   -0.493947   0.551791   0.000339
  7   6   0   -1.397617   1.614983   0.000358
  8   1   0   -3.480627   2.153672   0.000429
  9   1   0   -2.694876   -2.064066   0.001695
 10   1   0   -1.054438   2.640087   -0.000307
 11   6   0   0.202968   -1.739597   0.000037
 12   1   0   0.192781   -2.391588   0.876552
 13   6   0   1.397209   -0.811199   -0.002425
 14   6   0   2.742478   -1.129948   -0.004240
 15   6   0   3.696157   -0.098127   -0.005024
 16   6   0   3.261063   1.240724   -0.001011
 17   6   0   1.910386   1.555523   0.001223
 18   6   0   0.966646   0.528323   -0.001094
 19   1   0   3.069401   -2.162304   -0.006016
 20   1   0   3.998508   2.032768   -0.000265
 21   1   0   1.605245   2.593424   0.006717
 22   7   0   5.054875   -0.392874   -0.072206
 23   1   0   5.673369   0.327595   0.266162
 24   7   0   -4.578056   -0.226208   0.001253
 25   1   0   5.320453   -1.304708   0.265833
 26   6   0   -5.725118   -0.440540   0.001170

0503aac_mol1_CN_TD_B3LYP6311++2d2p_PCMdmso_opt.log

Standard orientation:
```
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type          X           Y           Z
---------------------------------------------------------------------
   1          1          0         0.200897   -2.419739   -0.875807
   2          6          0        -2.739970    1.369549    0.000123
   3          6          0        -3.222350    0.026135    0.000030
   4          6          0        -2.305624   -1.075055   -0.000017
   5          6          0        -0.962311   -0.802358   -0.000002
   6          6          0        -0.473954    0.541261    0.000038
   7          6          0        -1.393358    1.630144    0.000124
   8          1          0        -3.458595    2.176602    0.000211
   9          1          0        -2.687066   -2.086044   -0.000050
  10          1          0        -1.041683    2.652689    0.000231
  11          6          0         0.206030   -1.767403   -0.000058
  12          1          0         0.200962   -2.419756    0.875680
  13          6          0         1.403076   -0.840642   -0.000080
  14          6          0         2.731063   -1.146671   -0.000029
  15          6          0         3.690456   -0.086609    0.000010
  16          6          0         3.249916    1.263136   -0.000146
  17          6          0         1.906675    1.572430   -0.000185
  18          6          0         0.952351    0.521884   -0.000074
  19          1          0         3.075632   -2.172363    0.000006
  20          1          0         3.991227    2.050693   -0.000274
  21          1          0         1.590303    2.605431   -0.000338
  22          7          0         5.012021   -0.375680    0.000223
  23          1          0         5.705681    0.352930    0.000405
  24          7          0        -4.559649   -0.206813   -0.000009
  25          1          0         5.339420   -1.326799    0.000186
  26          6          0        -5.722565   -0.428500   -0.000026
---------------------------------------------------------------------
```

0801aaa_H2NPhPhNH2_b3lyp6311++2d2p_PCMdmso.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.740956	0.000931	-0.001901
2	6	0	-1.475236	-1.139397	-0.357755
3	6	0	-2.862887	-1.145429	-0.361552
4	6	0	-3.585757	0.000977	-0.007454
5	6	0	-2.864365	1.147148	0.350210
6	6	0	-1.476612	1.140829	0.352438
7	6	0	0.740956	0.000948	0.001870
8	6	0	1.475214	-1.139388	0.357761
9	6	0	2.862874	-1.145449	0.361514
10	6	0	3.585716	0.000937	0.007449
11	6	0	2.864383	1.147134	-0.350185
12	6	0	1.476620	1.140832	-0.352473
13	1	0	-0.954467	-2.039133	-0.656567
14	1	0	-3.394401	-2.042867	-0.651793
15	1	0	-3.396771	2.044829	0.638195
16	1	0	-0.956854	2.038659	0.658686
17	1	0	0.954407	-2.039087	0.656611
18	1	0	3.394356	-2.042959	0.651596
19	1	0	3.396801	2.044850	-0.638027
20	1	0	0.956902	2.038654	-0.658810
21	7	0	-4.981734	0.019508	-0.072161
22	1	0	-5.423198	-0.881083	0.034313
23	1	0	-5.423813	0.712748	0.511977
24	7	0	4.981808	0.019610	0.072313
25	1	0	5.423143	-0.881109	-0.034003
26	1	0	5.423664	0.712242	-0.512774

0801baa_H2NPhPhNH2_TD_b3lyp6311++2d2p_PCMdmso_sp.log

Standard orientation:

Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type   X   Y   Z
----
   1   6   0   -0.740956 -0.000931   0.001901
   2   6   0   -1.475236   1.139397   0.357755
   3   6   0   -2.862887   1.145429   0.361552
   4   6   0   -3.585757 -0.000977   0.007454
   5   6   0   -2.864365 -1.147148 -0.350210
   6   6   0   -1.476612 -1.140829 -0.352438
   7   6   0   0.740956 -0.000948 -0.001870
   8   6   0   1.475214   1.139388 -0.357761
   9   6   0   2.862874   1.145449 -0.361514
  10   6   0   3.585716 -0.000937 -0.007449
  11   6   0   2.864383 -1.147134   0.350185
  12   6   0   1.476620 -1.140832   0.352473
  13   1   0   -0.954467   2.039133   0.656567
  14   1   0   -3.394401   2.042867   0.651793
  15   1   0   -3.396771 -2.044829 -0.638195
  16   1   0   -0.956854 -2.038659 -0.658686
  17   1   0   0.954407   2.039087 -0.656611
  18   1   0   3.394356   2.042959 -0.651596
  19   1   0   3.396801 -2.044850   0.638027
  20   1   0   0.956902 -2.038654   0.658810
  21   7   0   -4.981734 -0.019508   0.072161
  22   1   0   -5.423198   0.881083 -0.034313
  23   1   0   -5.423813 -0.712748 -0.511977
  24   7   0   4.981808 -0.019610 -0.072313
  25   1   0   5.423143   0.881109   0.034003
  26   1   0   5.423664 -0.712242   0.512774

0801caa_H2NPhPhNH2_TD_b3lyp6311++2d2p_PCMdmso_opt.log

Standard orientation:

Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type   X   Y   Z
----
   1   6   0   -0.704912 -0.000534   0.000149
   2   6   0   -1.484094 -1.224722 -0.001654
   3   6   0   -2.854014 -1.215204 -0.004724
   4   6   0   -3.582903   0.000467 -0.001998
   5   6   0   -2.853914   1.215117 -0.004853
   6   6   0   -1.483534   1.224822 -0.001846
   7   6   0   0.704923 -0.000523   0.000402
   8   6   0   1.484105 -1.224677   0.002211
   9   6   0   2.853986 -1.215198   0.004798
  10   6   0   3.582933   0.000546   0.001627
  11   6   0   2.853952   1.215160   0.004956
  12   6   0   1.483555   1.224861   0.002462
  13   1   0   -0.984472 -2.180774   0.002910
  14   1   0   -3.396154 -2.152867 -0.008520
  15   1   0   -3.395888   2.152928 -0.008784
  16   1   0   -0.983637   2.180641   0.002785
  17   1   0   0.984454 -2.180717 -0.001793
  18   1   0   3.396195 -2.152816   0.008745
  19   1   0   3.395880   2.152997   0.008830
  20   1   0   0.983653   2.180675 -0.001804
  21   7   0   -4.963433 -0.000045 -0.061165
  22   1   0   -5.439751 -0.842859   0.221083
  23   1   0   -5.440326   0.843235   0.218657
  24   7   0   4.963326 -0.000128   0.059668
  25   1   0   5.439738 -0.843143 -0.221617
  26   1   0   5.440552   0.843221 -0.219194

0831aaa_CNPhPhNH2_b3lyp6311++2d2p_PCMdmso.log

Standard orientation:

Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type   X   Y   Z
----
   1   6   0   -0.986573   0.000460 -0.001752
   2   6   0   -1.718515 -1.148141 -0.336250
   3   6   0   -3.103963 -1.152428 -0.342806
   4   6   0   -3.825948   0.001479 -0.004790
   5   6   0   -3.103997   1.154428   0.336458
   6   6   0   -1.718487   1.148993   0.333183
   7   6   0   0.492057   0.000087 -0.000351
   8   6   0   1.218855 -1.150554   0.344958
   9   6   0   2.604235 -1.159973   0.345898
  10   6   0   3.298252 -0.000344   0.001299
  11   6   0   2.605032   1.159506 -0.344051
  12   6   0   1.219626   1.150506 -0.344768
  13   1   0   -1.198975 -2.052958 -0.620224
  14   1   0   -3.636659 -2.052909 -0.619770
  15   1   0   -3.636415   2.055240   0.613041
  16   1   0   -1.198804   2.051661   0.623672
  17   1   0   0.695274 -2.048655   0.638686
  18   1   0   3.149765 -2.050583   0.620817
  19   1   0   3.151162   2.049916 -0.618425
  20   1   0   0.696597   2.048638 -0.639379
  21   7   0   -5.214735   0.018895 -0.066213
  22   1   0   -5.667265 -0.876877   0.027868
  23   1   0   -5.666972   0.730152   0.486590
  24   7   0   4.687024 -0.000642   0.001948
  25   6   0   5.853806 -0.000918   0.002469

0831baa_CNPhPhNH2_TD_b3lyp6311++2d2p_PCMdmso_sp.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.986573	-0.000460	-0.001752
2	6	0	1.718515	1.148141	-0.336250
3	6	0	3.103963	1.152428	-0.342806
4	6	0	3.825948	-0.001479	-0.004790
5	6	0	3.103997	-1.154428	0.336458
6	6	0	1.718487	-1.148993	0.333183
7	6	0	-0.492057	-0.000087	-0.000351
8	6	0	-1.218855	1.150554	0.344958
9	6	0	-2.604235	1.159973	0.345898
10	6	0	-3.298252	0.000344	0.001299
11	6	0	-2.605032	-1.159506	-0.344051
12	6	0	-1.219626	-1.150506	-0.344768
13	1	0	1.198975	2.052958	-0.620224
14	1	0	3.636659	2.052909	-0.619770
15	1	0	3.636415	-2.055240	0.613041
16	1	0	1.198804	-2.051661	0.623672
17	1	0	-0.695274	2.048655	0.638686
18	1	0	-3.149765	2.050583	0.620817
19	1	0	-3.151162	-2.049916	-0.618425
20	1	0	-0.696597	-2.048638	-0.639379
21	7	0	5.214735	-0.018895	-0.066213
22	1	0	5.667265	0.876877	0.027868
23	1	0	5.666972	-0.730152	0.486590
24	7	0	-4.687024	0.000642	0.001948
25	6	0	-5.853806	0.000918	0.002469

0831caa_CNPhPhNH2_TD_b3lyp6311++2d2p_PCMdmso_opt.log

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-0.971152	-0.000007	-0.000076
2	6	0	-1.734185	-1.213564	-0.066825
3	6	0	-3.103713	-1.216194	-0.066898
4	6	0	-3.832879	0.000005	0.000053
5	6	0	-3.103695	1.216202	0.066888
6	6	0	-1.734168	1.213559	0.066684
7	6	0	0.469887	-0.000009	-0.000074
8	6	0	1.228093	-1.216640	0.066037
9	6	0	2.598600	-1.223581	0.070377
10	6	0	3.320828	-0.000001	0.000019
11	6	0	2.598596	1.223574	-0.070414
12	6	0	1.228090	1.216624	-0.066163
13	1	0	-1.228095	-2.163087	-0.130996
14	1	0	-3.642947	-2.152111	-0.123029
15	1	0	-3.642910	2.152130	0.123029
16	1	0	-1.228063	2.163079	0.130766
17	1	0	0.723340	-2.168185	0.130134
18	1	0	3.142233	-2.155450	0.129537
19	1	0	3.142226	2.155445	-0.129567
20	1	0	0.723334	2.168164	-0.130325
21	7	0	-5.184019	0.000014	0.000064
22	1	0	-5.706704	-0.858460	-0.044805
23	1	0	-5.706699	0.858450	0.045703
24	7	0	4.679743	0.000006	0.000084
25	6	0	5.861402	0.000013	0.000144