Supplementary Information:

Design, Synthesis and Proticity Inclined Conformational Modulation in a Highly Fluorescent Bichromophoric Naphthalimide Derivative: Hint Directed from RICT Perspective

Ritika Joshi, Oinam Romesh Meitei[†], Himank Kumar, Manojkumar Jadhao and Sujit Kumar Ghosh[*]

Department of Chemistry, Visvesvaraya National Institute of Technology, Nagpur, Maharashtra, 440010, India

[†]The present address of this author (O.R.M.) is as follows:

Lehrstuhl für Theoretische Chemie,

Friedrich-Alexander Universität Erlangen-Nürnberg,

Egerlandstraße 3, 91058 Erlangen, Germany

Corresponding Author

Dr. Sujit Kumar Ghosh, Department of Chemistry, Visvesvaraya National Institute of Technology, Nagpur, Maharashtra, PIN- 440010, India, e-mail: sujitju@yahoo.co.in, skghosh@chm.vnit.ac.in, Phone no: +(91) 712 2801775, Fax: + (91) 712-2223230/2801357

Supplementary Information Legends:

Figure S1: Emission spectra of CBIQD in chloroform at 298K exciting at (i) peak b (333 nm) and (ii) peak a (348 nm).

Figure S2: Design of several naphthalimide derivatives to streamline the synthesis

Table S1: Energetics of different designed naphthalimide derivatives with DNA (PDB ID: 1Z3F)

Table S2: Photophysical parameters of CBIQD in different solvents at 298 K

Table S3: Mulliken atomic charge analysis of CBIQD in ground and excited states

Figure S1: Emission spectra of CBIQD in chloroform at 298K exciting at (i) peak b (333 nm) and (ii) peak a (348 nm)

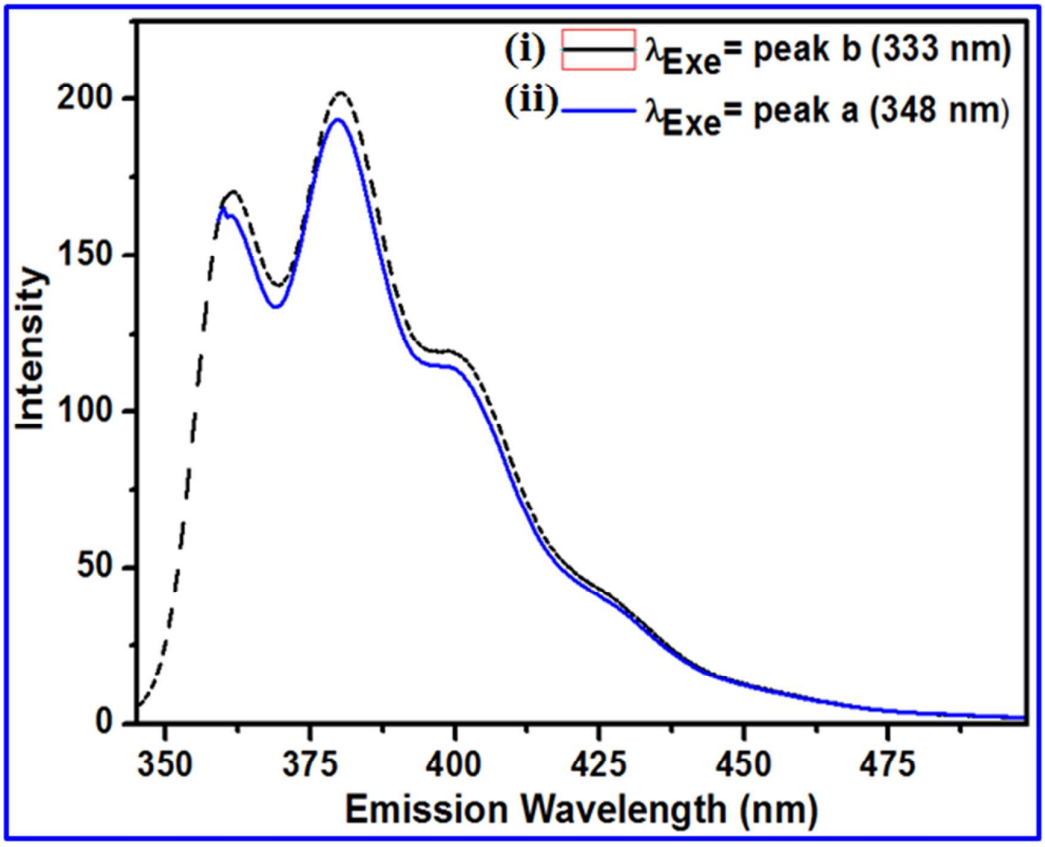

Figure S2: Design of several naphthalimide derivatives to streamline the synthesis

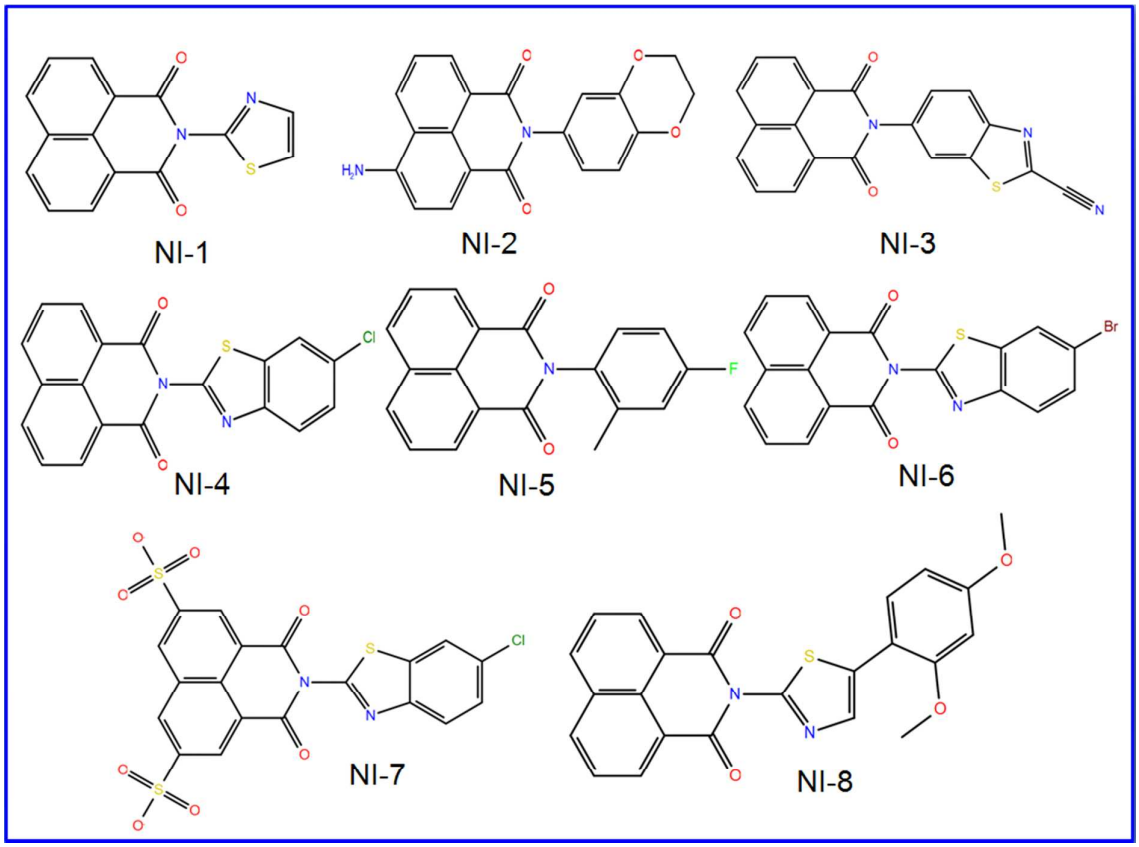

Table S1: Energetics of different naphthalimide derivatives with DNA (PDB ID: 1Z3F)

Entry Name	XP GScore	Glide Score/ kcal/mol	Glide emodel
NI-1	-6.12	-6.12	-54.24
NI-2	-5.62	-5.62	-52.90
NI-3	-5.55	-5.55	-54.42
NI-4(CBIQD)	**-5.36**	**-5.36**	**-59.28**
NI-5	-5.07	-5.07	-50.84
NI-6	-4.89	-4.88	-57.66
NI-7	-3.92	-3.92	-50.89
NI-8	-0.59	-0.59	-60.97

Table S2: Photophysical parameters of CBIQD in different solvents at 298 K

Solvent	$E_T(30)$/ kcal/mol	Absorbance/nm		Fluorescence bands/nm		$\Delta\bar{\nu}$/cm^{-1}
		Peak 'b' λ_{abs}^{max}	Peak 'a'	Probable LE band	CT band λ_{em}^{max}	
Cyhx	30.9	328	343	362	-	2863
Hex	31.0	326	343	367	-	3427
Hept	31.1	326	343	367	-	3427
Diox	36.0	331	344	363	374	3474
THF	37.4	332	346	367	376	3525
Chloro	39.1	333	348	362	379	3645
DCM	40.7	334	347	360	378	3485
ACN	45.6	331	344	360	378	3757
^{n}OcOH	48.1	333	343	366	384	3988
^{i}PrOH	48.4	333	343	367	384	3988
^{n}BuOH	49.7	333	343	368	385	4056
EtOH	51.9	333	343	369	385	4056
MeOH	55.4	332	343	371	386	4214
Water	63.1	344	-	383	397	3881

Table S3: Mulliken atomic charge analysis of CBIQD in ground and excited states

Local population analysis gives a quantitative idea of the electronic charge at the local site and is estimated with the help of Mulliken partial atomic charges given in the following table (refer atom numbering included in the following figure). In GS the sum of partial atomic charges for the NI ring is negative while that for BT ring is positive. This is further supported by the distribution of HOMO which is more concentrated on the NI ring. In the S_1 state, the sum of atomic charges on the NI ring became more negative as compared to the GS and the sum of atomic charges for BT ring became more positive. This gives a clear indication that the NI ring acts as an acceptor and BT ring as a donor moiety upon excitation of CBIQD.[1]

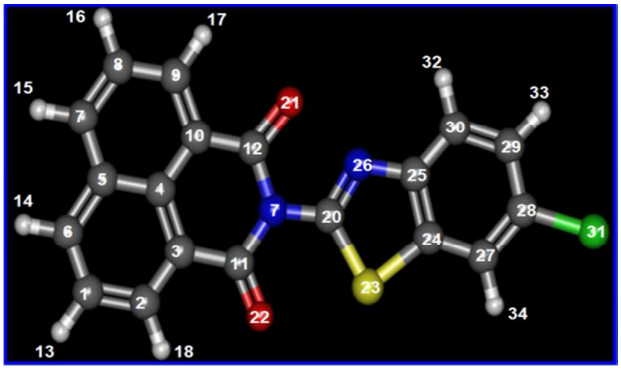

Figure: Structure of CBIQD with atom numbering

Table: Mulliken atomic charge analysis of CBIQD in ground and excited states

Ground State				Excited State			
Naphthalimide ring		Benzothiazole ring		Naphthalimide ring		Benzothiazole ring	
1C	-0.141	20C	0.120	1C	-0.145	20C	0.217
2C	-0.154	23S	0.491	2C	-0.153	23S	0.633
3C	0.016	24C	-0.281	3C	0.001	24C	-0.315
4C	0.066	25C	0.156	4C	0.048	25C	0.219
5C	0.033	26N	-0.294	5C	0.033	26N	-0.400
6C	-0.137	27C	-0.136	6C	-0.154	27C	-0.145
7C	-0.137	28C	-0.239	7C	-0.161	28C	-0.238
8C	-0.141	29C	-0.128	8C	-0.145	29C	-0.134
9C	-0.154	30C	-0.065	9C	-0.173	30C	-0.046
10C	0.016	31Cl	0.073	10C	0.070	31Cl	0.081
11C	0.508	32H	0.177	11C	0.496	32H	0.187
12C	0.508	33H	0.181	12C	0.445	33H	0.186
13H	0.162	34H	0.197	13H	0.151	34H	0.202
14H	0.167			14H	0.155		
15H	0.167			15H	0.144		
16H	0.162			16H	0.144		
17H	0.193			17H	0.164		
18H	0.193			18H	0.180		
19N	-0.761			19N	-0.750		
21O	-0.408			21O	-0.358		
22O	-0.408			22O	-0.438		
SUM	-0.25	SUM	0.252	SUM	-0.446	SUM	0.447

SUPPORTING REFERENCES

(1) Dhas, D. A.; Joe, I. H.; Roy, S. D. D.; Freeda, T. H. DFT Computations and Spectroscopic Analysis of a Pesticide: Chlorothalonil. *Spectrochim. Acta. A. Mol. Biomol. Spectrosc.***2010**, *77*, 36–44.