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The optical signature of 2,6-bis((E)-2-(benzoxazol-2-yl)vinyl)naphthalene (BBVN) laser dye: A TDDFT Study

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Table S1 Some selected structural parameters for the BBVN laser dye in both ground (GS) and first excited (ES) singlet states with the corresponding Mulliken atomic charges computed at the BMK/cc-pvdz level of theory in gas phase.

	GS (S_0)	ES (S_1)	Atom	Atomic charge	
				S_0	S_1
Bond length (Å)					
C4-C5	1.4079	1.4167	C1	-0.016	-0.018
C4-N7	1.3906	1.3756	C2	-0.015	-0.014
C5-O9	1.3570	1.3524	C3	-0.037	-0.036
N7-C8	1.3023	1.3188	C4	0.025	0.027
C8-C10	1.4536	1.4278	C5	0.150	0.149
C10-C11	1.3525	1.3827	C6	-0.056	-0.057
C11-C12	1.4721	1.4331	N7	-0.246	-0.247
C12-C13	1.3924	1.4305	C8	0.244	0.249
C13-C14	1.4208	1.3950	O9	-0.228	-0.228
C14-C15	1.4362	1.4519	C10	-0.069	-0.074
C15-C21	1.4208	1.3951	C11	0.033	0.025
C21-C20	1.3926	1.4323	C12	0.054	0.054
C20-C22	1.4710	1.4285	C13	-0.057	-0.062
C22-C23	1.3521	1.3870	C14	0.054	0.064
C23-C24	1.4570	1.4261	C15	0.056	0.067
C24-N28	1.3018	1.3219	C16	-0.023	-0.025
N28-C27	1.3888	1.3716	C17	-0.027	-0.023
C27-C26	1.4085	1.4186	C18	-0.023	-0.024
Bond angles (°)			C19	-0.025	-0.022
C4-N7-C8	104.07	104.36	C20	0.055	0.058
C5-O9-C8	104.68	104.80	C21	-0.059	-0.064
C8-C10-C11	123.31	123.49	C22	0.047	0.038
C10-C11-C12	126.71	125.90	O23	-0.085	-0.092
Torsional angles (°)			C24	0.248	0.256
O9-C8-C10-C11	0.0	0.0	O25	-0.226	-0.226
C8-C10-C11-C12	-180.0	-180.0	C26	0.143	0.141
C10-C11-C12-C13	0.0	0.0	C27	0.038	0.040
			N28	-0.251	-0.254
Dipole Moment (D)	2.21	2.20	C29	-0.055	-0.056
			C30	-0.017	-0.019
			C31	-0.015	-0.014
			C32	-0.041	-0.039

Fig. S1 Molecular structures of EE-, EZ-, and ZZ-BBVN isomers.

Table S2 Dipole moments and dipole moment shifts (ΔD, in Debye) upon photon absorption(abs) and emission(fl) obtained for BBVN at the BMK/cc-pvdz level at the optimal geometry of the ground state (GS) and excited state (ES) in the corresponding solvent.

Dipole Moment	**Gas phase**	**Dioxane** ε=2.2099	**Acetone** 20.493	**MeOH** 32.613	**CH_3CN** 35.688
S_0(GS)	2.21	2.64	3.41	3.43	3.48
S'(GS)	2.38	2.86	3.51	3.53	3.58
S_1(ES)	2.20	2.92	3.87	3.89	3.96
S'_0(ES)	2.20	2.64	3.44	3.45	3.51
$^{a}\Delta D(GS)^{abs}$	0.17	0.22	0.10	0.10	0.10
$^{b}\Delta D(ES)^{fl}$	0.0	0.28	0.43	0.44	0.45
$^{c}\Delta\Delta D^{fl\text{-}abs}$		0.06	0.33	0.34	0.35

$^{a}\Delta D(GS)^{abs} = S'_1(GS) - S_0(GS)$, $^{b}\Delta D(ES)^{fl} = S_1(ES) - S'_0(ES)$, $^{c}\Delta\Delta D^{fl\text{-}abs} = \Delta D(ES)^{fl} - \Delta D(GS)^{abs}$