

Paying Comprehensive Attention to the Temperature-Dependent Dual-Channel Excited-State
Intramolecular Proton Transfer Mechanism of Fluorescence Ratio Probe BZ-DAM

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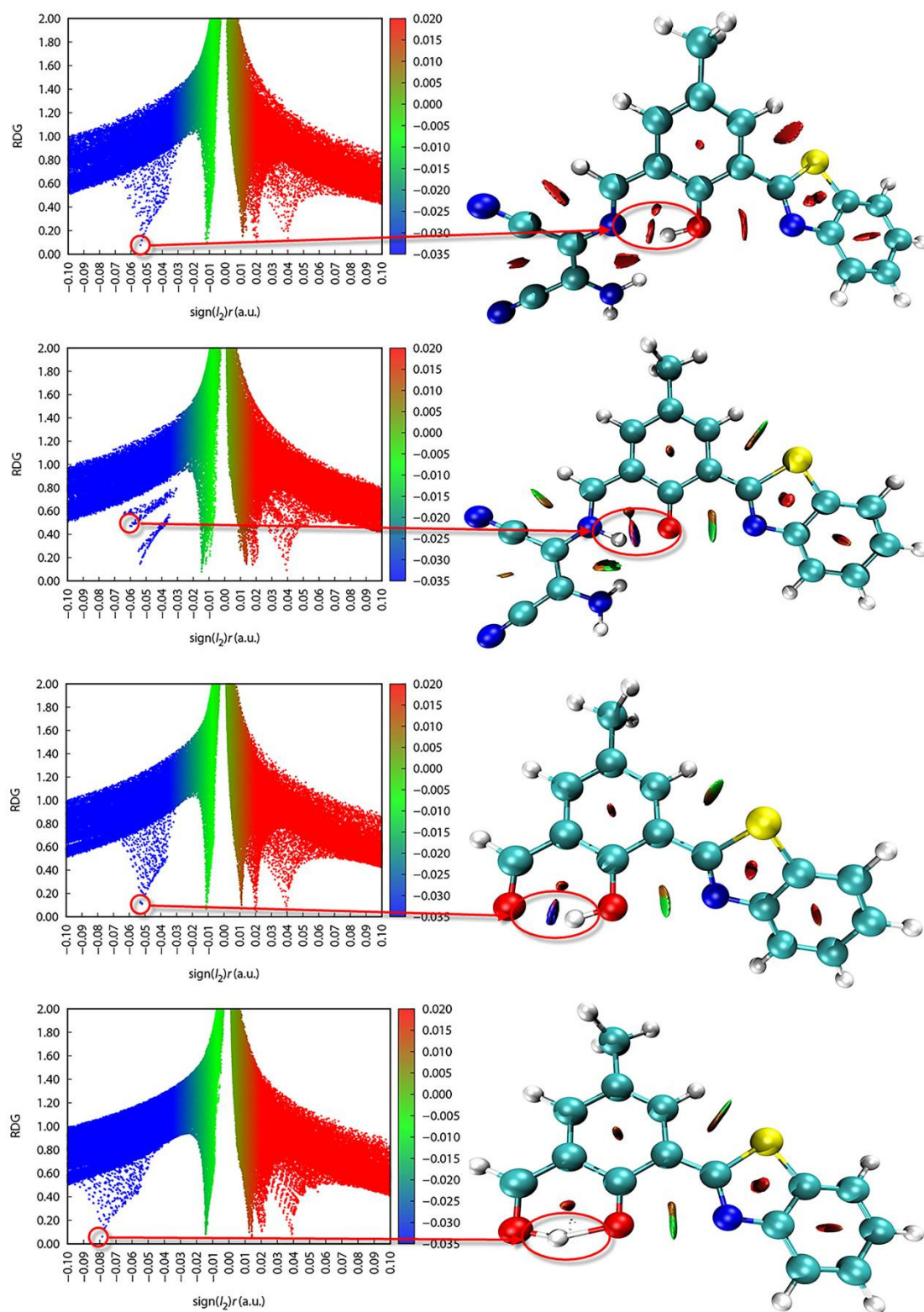
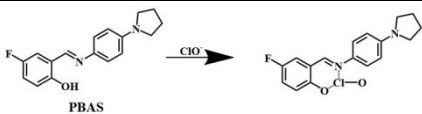
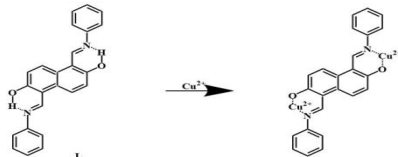
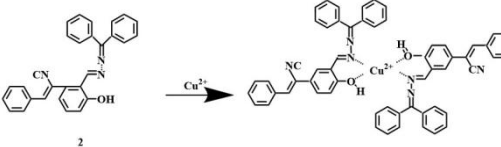
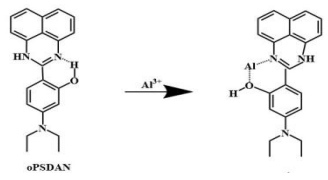
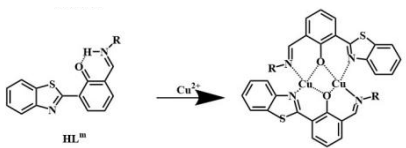
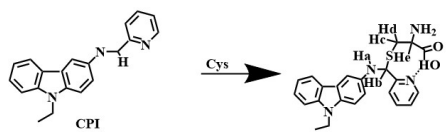
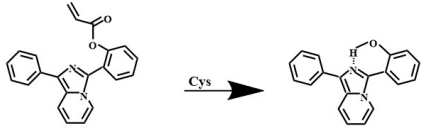
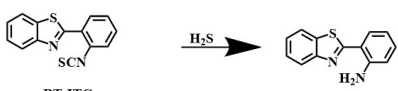
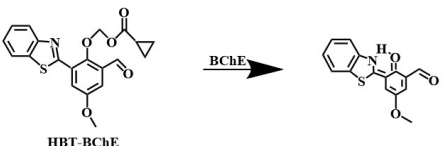




Figure S1. RDG versus $\text{Sign}(\lambda_2) \rho(r)$ scatter plots of BZ-DAM and BZ-CHO in channel 2 in the S_0 and S_1 states.

Table S1 The structures and properties of three kinds of fluorescent probes reported are compared.

type	Probes	Detection mechanism	Ref.
"turn-off" fluorescent probe	 <p>PBAS</p>	Reduction in fluorescence intensity	J Fluoresc. 2019 , 29, 399-406
	 <p>L</p>	Reduction in fluorescence intensity	Molecules. 2021 , 26, 1-11
	 <p>2</p>	fluorescence quenching	Inorg. Chem. Commun. 2023 , 152, 110640
	 <p>oPSDAN</p>	fluorescence quenching	Spectrochim. Acta. Part A. 2023 , 293, 122471
	 <p>HL³ⁿ</p>	fluorescence quenching	Spectrochim. Acta. Part A. 2023 , 287, 122051
"turn-on" fluorescent probe	 <p>CPI</p>	increase in fluorescence intensity	Analytical Bioanalytical Chem. 2019 , 411, 6203–6212
	 <p>MZC-AC</p>	increase in fluorescence intensity	ACS Omega. 2020 , 5, 19695–19701
	 <p>BT-ITC</p>	increase in fluorescence intensity	Spectrochim. Acta. Part A. 2022 , 278, 121333z
	 <p>HBT-BChE</p>	increase in fluorescence intensity	Spectrochim. Acta. Part A. 2023 , 287, 122044
	 <p>SNCN-AE</p>	increase in fluorescence intensity	Sens. Actuators B Chem. 2023 , 380, 133392
	 <p>SNC-AE</p>	increase in fluorescence intensity	


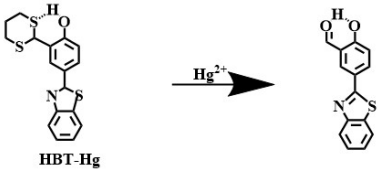

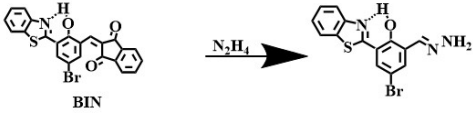
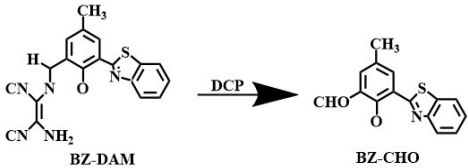
type	Probes	Detection mechanism	Ref.
Ratio fluorescence probe	 <p>Naph-1</p>	increase in fluorescence intensity	Analyst. 2019 , 144, 6922
	 <p>HBT-Hg</p>	Fluorescence red-shift	Spectrochim. Acta. Part A. 2020 , 243, 118817
	 <p>BTMSP</p>	Fluorescence blue-shift	Theor Chem Acc. 2022 , 141, 57
	 <p>BIN</p>	Fluorescence blue-shift	Anal. Chim. Acta. 2022 , 1227, 340320
	 <p>BZ-DAM</p>	Fluorescence blue-shift	New J. Chem. 2023 , 47, 250

Table S2 Calculated transition properties of BZ-DAM and BZ-CHO in ACN solvent at the TD-DFT/mpw1pw91/6-31g (d, p) theoretical level.

	transition	$\lambda_{\text{abs}}(\text{nm})$	f	Composition	CI (%)
channel 1	$S_0 \rightarrow S_1$	397.15	0.6100	H \rightarrow L	64.20%
	$S_0 \rightarrow S_2$	342.38	0.3723	H-1 \rightarrow L	65.03%
	$S_0 \rightarrow S_3$	337.50	0.0677	H \rightarrow L+1	68.06%
	$S_0 \rightarrow S_4$	309.68	0.4493	H-1 \rightarrow L+1	66.94%
	$S_0 \rightarrow S_5$	298.45	0.0003	H-4 \rightarrow L	67.56%
	$S_0 \rightarrow S_6$	297.15	0.0772	H-2 \rightarrow L	64.82%
	$S_0 \rightarrow S_1$	345.78	0.4650	H \rightarrow L	69.33%
	$S_0 \rightarrow S_2$	333.43	0.0000	H-3 \rightarrow L	51.68%
	$S_0 \rightarrow S_3$	292.50	0.0396	H-1 \rightarrow L	58.32%
	$S_0 \rightarrow S_4$	285.48	0.2130	H \rightarrow L+1	45.52%
	$S_0 \rightarrow S_5$	276.51	0.0839	H-2 \rightarrow L+1	51.72%
	$S_0 \rightarrow S_6$	268.22	0.0001	H-3 \rightarrow L+1	49.82%
channel 2	$S_0 \rightarrow S_1$	399.81	0.6100	H \rightarrow L	66.28%
	$S_0 \rightarrow S_2$	350.61	0.5187	H-1 \rightarrow L	66.71%
	$S_0 \rightarrow S_3$	323.33	0.0012	H-2 \rightarrow L	69.92%
	$S_0 \rightarrow S_4$	309.98	0.1207	H \rightarrow L+1	65.72%
	$S_0 \rightarrow S_5$	298.23	0.0353	H-3 \rightarrow L	63.81%
	$S_0 \rightarrow S_6$	287.25	0.3763	H-1 \rightarrow L+1	65.42%
	$S_0 \rightarrow S_1$	346.36	0.2692	H \rightarrow L	69.37%
	$S_0 \rightarrow S_2$	305.02	0.0006	H-3 \rightarrow L	55.00%
	$S_0 \rightarrow S_3$	299.94	0.0094	H-1 \rightarrow L	66.56%
	$S_0 \rightarrow S_4$	285.00	0.2161	H \rightarrow L+1	56.15%
	$S_0 \rightarrow S_5$	282.60	0.1481	H-2 \rightarrow L	55.75%
	$S_0 \rightarrow S_6$	265.35	0.0312	H-1 \rightarrow L+1	63.46%

Table S3 Indexes characterizing the distribution of choles and celes of BZ-DAM and BZ-CHO.

	D(Å)	Sm	Sr	H(Å)	t(Å)
BZ-DAM-S ₁	0.658	0.476	0.751	3.545	-1.987
BZ-DAM-S ₁ '	1.507	0.387	0.673	3.744	-1.451
BZ-CHO-S ₁	0.242	0.407	0.675	3.159	-1.329
BZ-CHO-S ₁ '	1.135	0.381	0.684	2.909	-1.148
BZ-DAM-1-S ₁	3.960	0.276	0.595	3.399	1.441
BZ-CHO-1-S ₁	2.525	0.364	0.678	2.958	0.150