Electronic Supplementary Information

Computational design of *p*-(dimethylamino)benzylidene-derived push-pull polyenes with high first-hyperpolarizabilities

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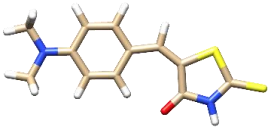
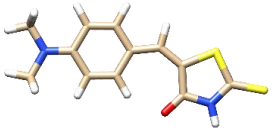
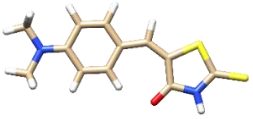
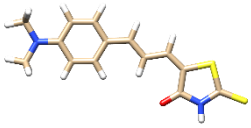
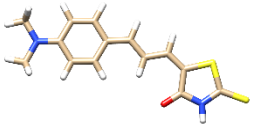
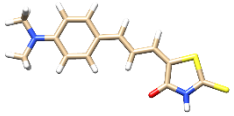
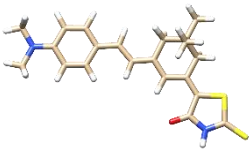
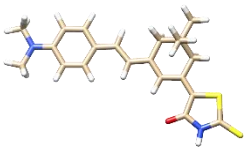
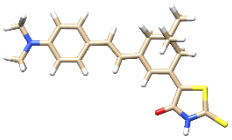
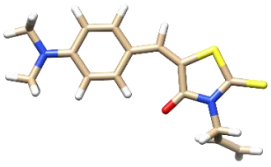
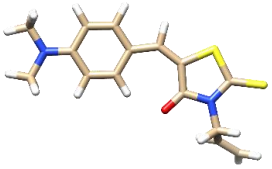
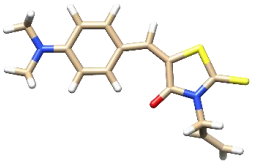
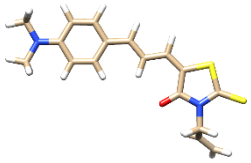
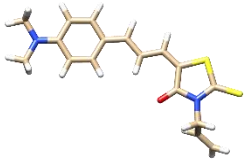
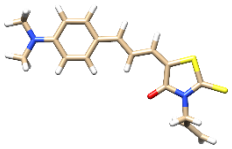
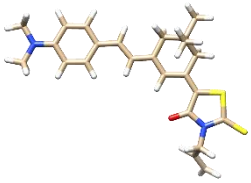
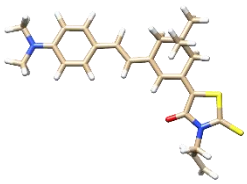
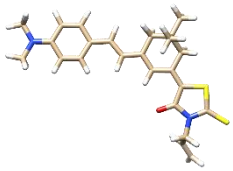
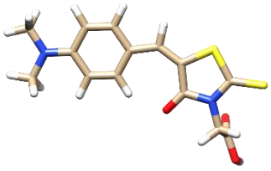
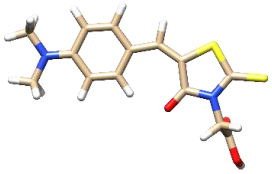
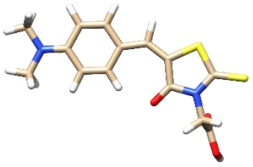
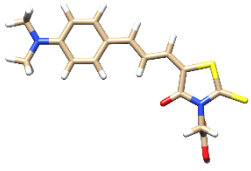
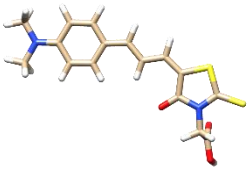
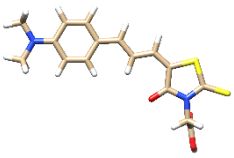
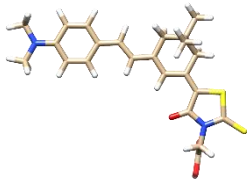
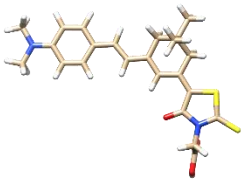
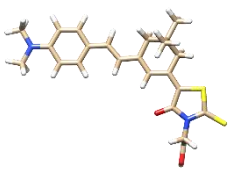
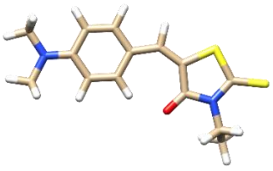
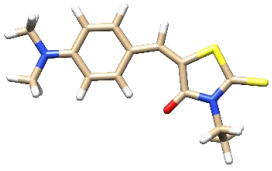
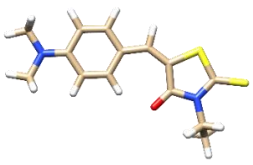
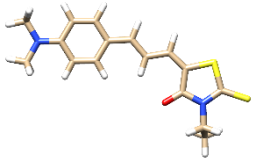
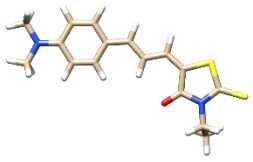
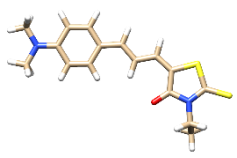
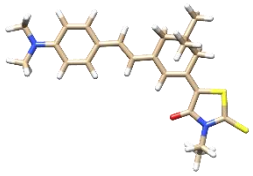
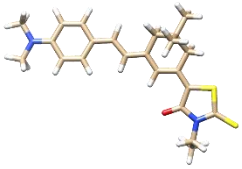
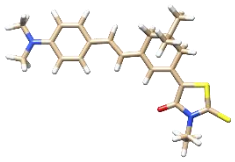
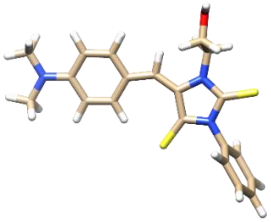
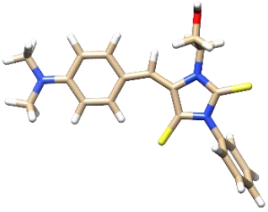
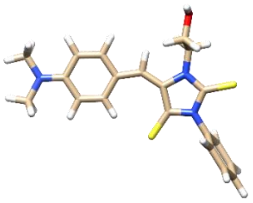
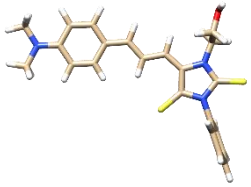
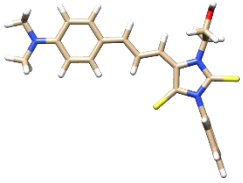
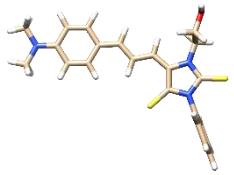
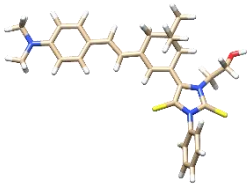
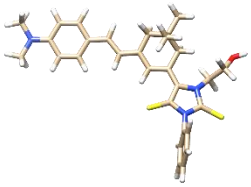
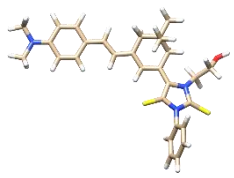
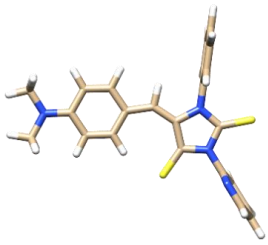
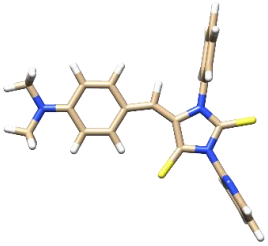
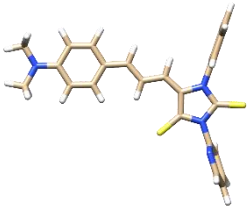
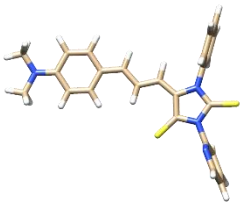
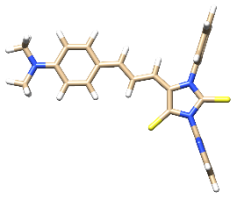
	Gas phase	Chloroform	Methanol
R1-1			
R1-2			
R1-3			
R2-1			
R2-2			
R2-3			
R3-1			
R3-2			
R3-3			

	Gas phase	Chloroform	Methanol
R4-1			
R4-2			
R4-3			
H1-1			
H1-2			
H1-3			
H2-1			
H2-2			

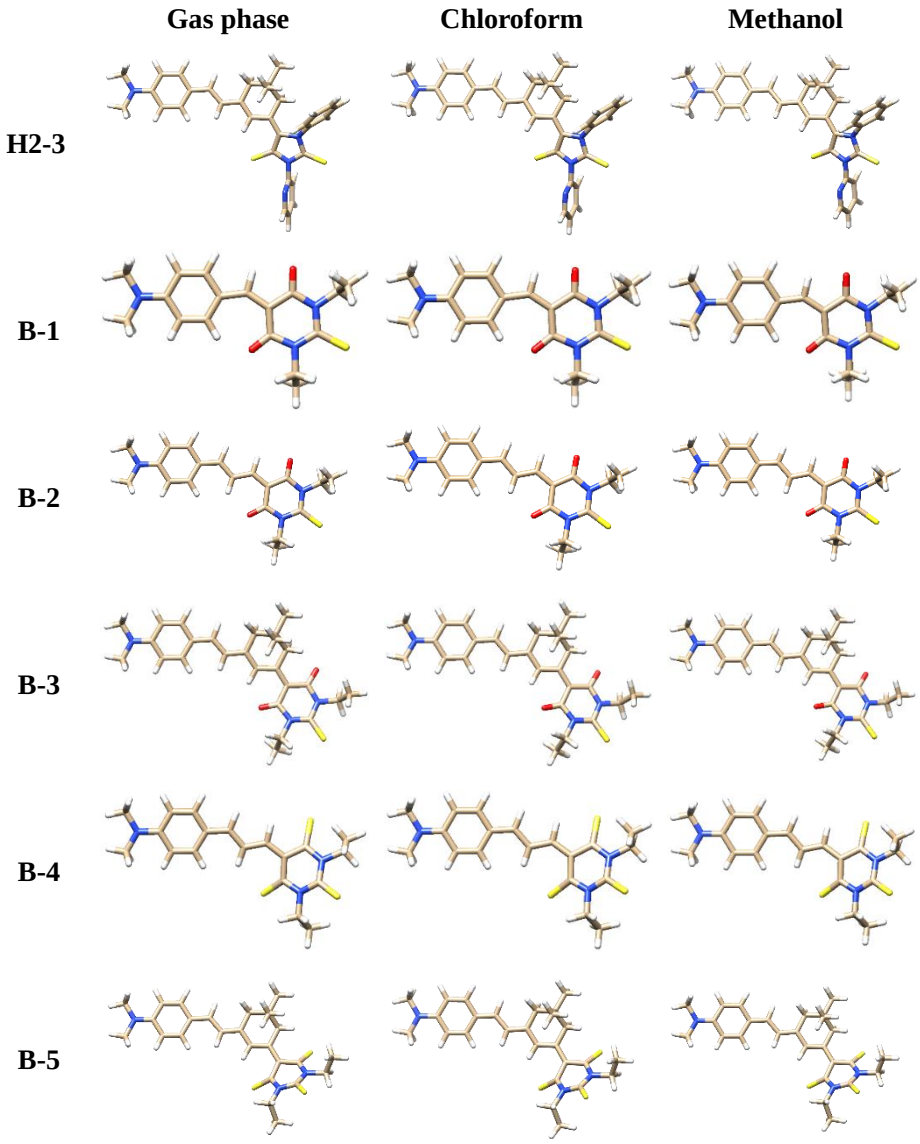


Figure S1. Geometries of the R-series, H-series, and B-series optimized at the B3LYP/6-31G** level in gas phase, chloroform, and methanol, respectively.

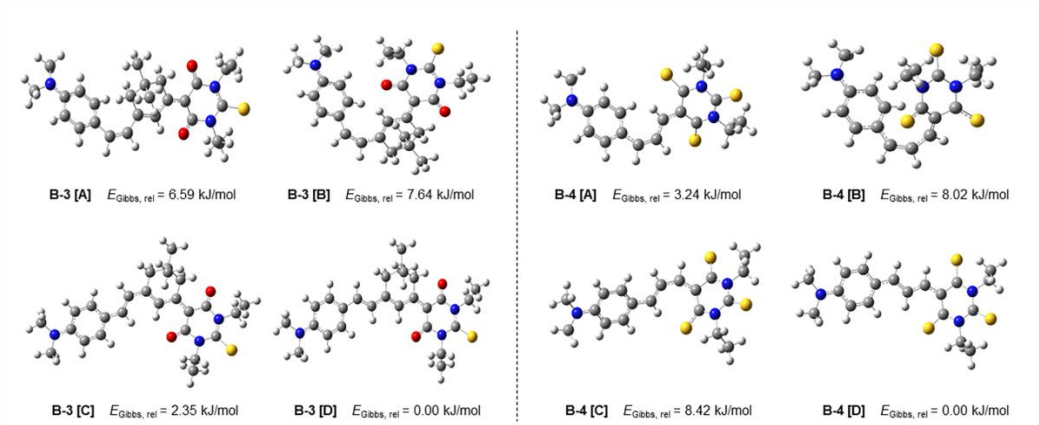


Figure S2. Optimized isomers of representative compounds B-3 and B-4 at the B3LYP/6-31G** level. The electron energies ($E_{M06\text{-}2X, elec}$) of all the isomers were calculated at the M06-2X/6-311G* level, whereas the thermal corrections ($E_{B3LYP, corr}$) to the Gibbs free energies (E_{Gibbs}) were performed at the B3LYP/6-31G** level, corresponding to the geometry optimization level. The E_{Gibbs} is then obtained according to $E_{Gibbs} = E_{M06\text{-}2X, elec} + E_{B3LYP, corr}$. The isomer with the lowest E_{Gibbs} value was reset to zero in each system, and the relative Gibbs free energies ($E_{Gibbs, rel}$) were given below the molecular stereograms.

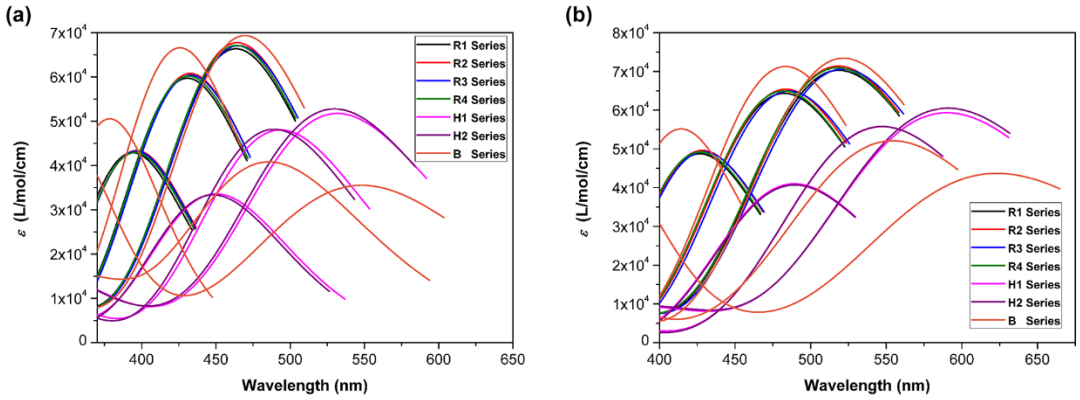
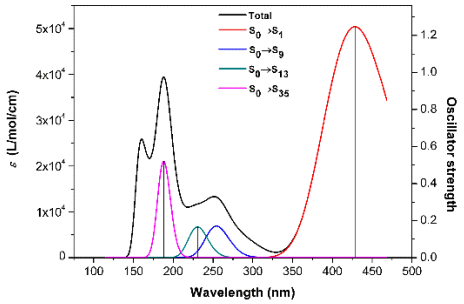
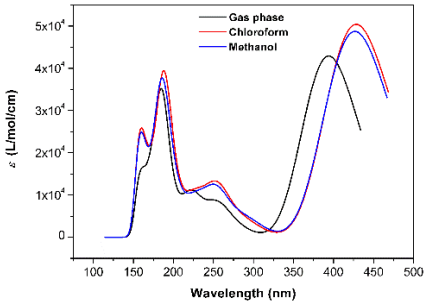
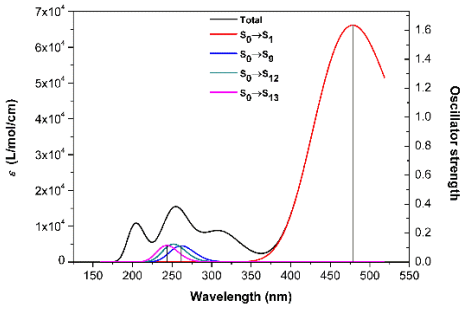
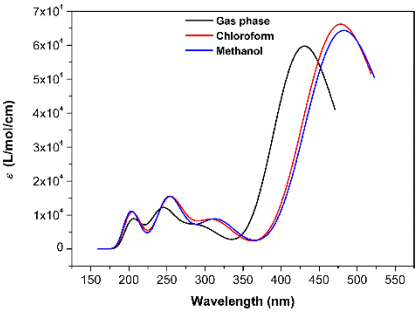
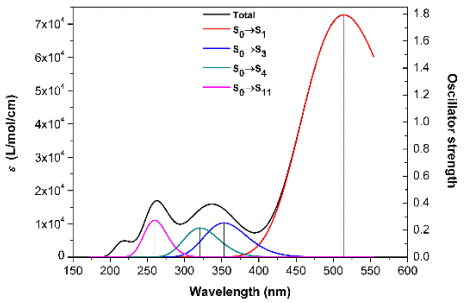
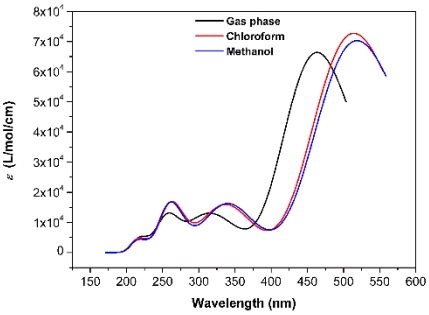
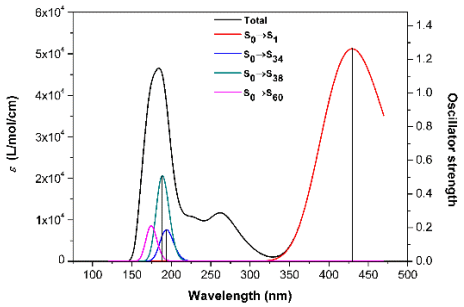
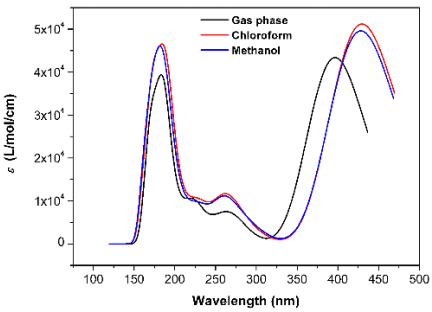
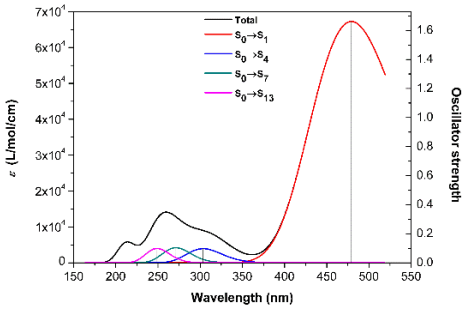


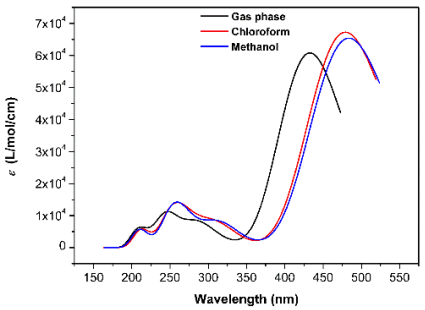
Figure S3. Calculated UV-Vis absorption spectra of the R-series, H-series, and B-series in (a) gas phase and (b) methanol.

	(a) Contribution of the crucial states	(b) Comparison in different media
R1-1		
R1-2		
R1-3		
R2-1		

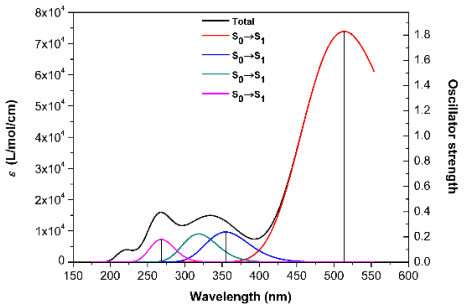
(a) Contribution of the crucial states **(b) Comparison in different media**

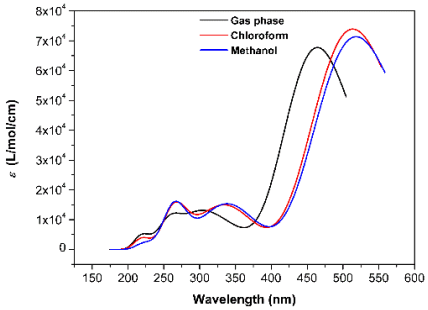
R2-2



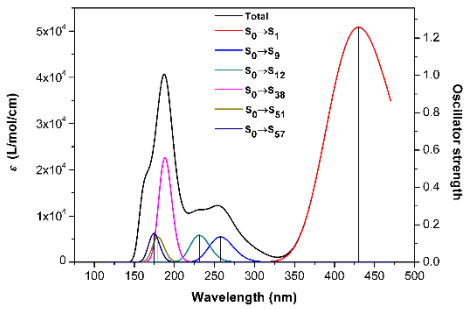


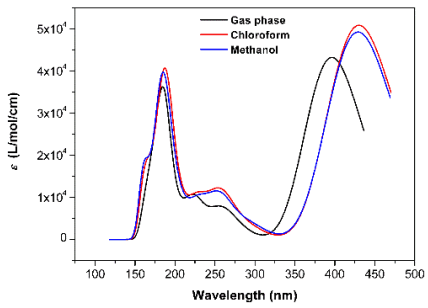
R2-3



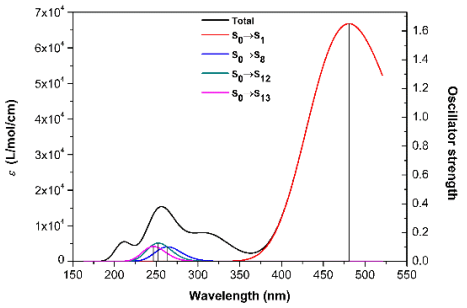


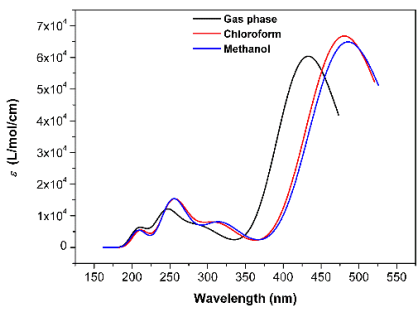
R3-1





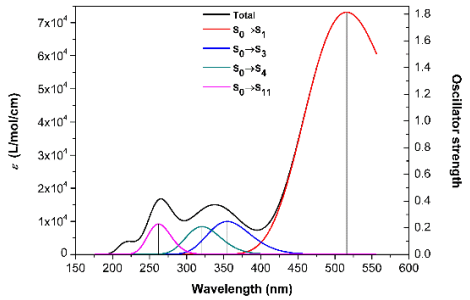
R3-2

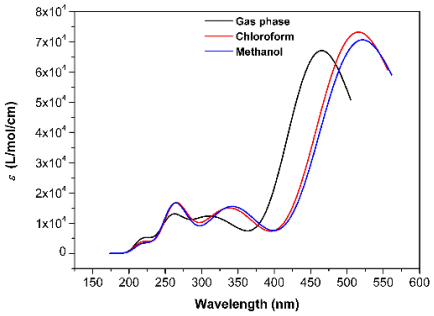




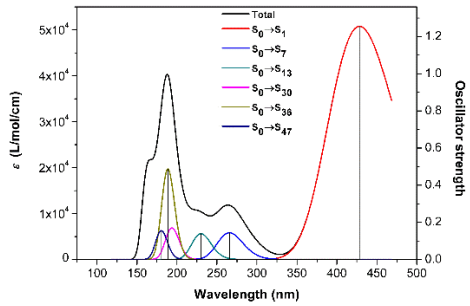
(a) Contribution of the crucial states **(b) Comparison in different media**

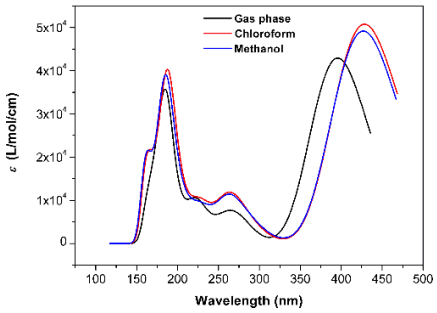
R3-3



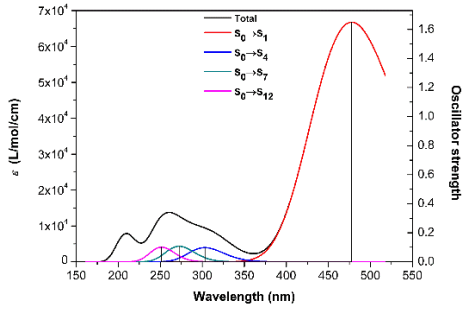


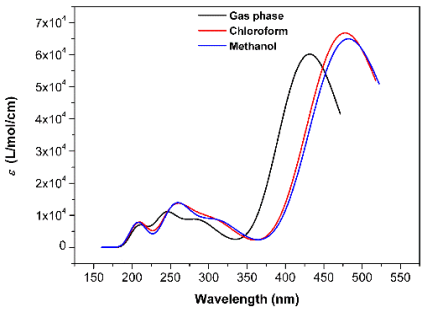
R4-1



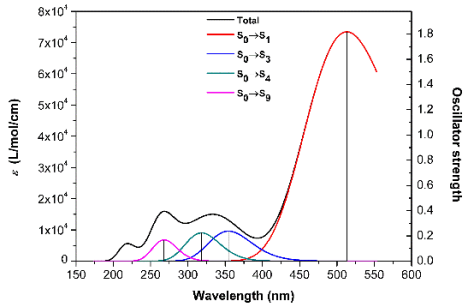


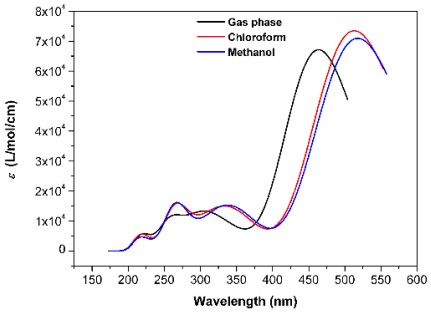
R4-2





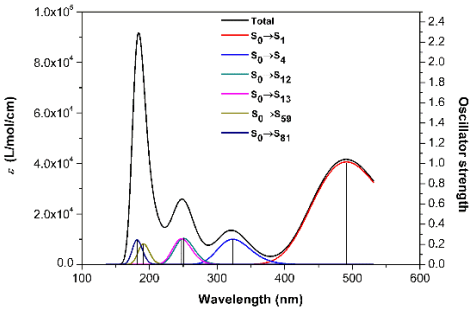
R4-3

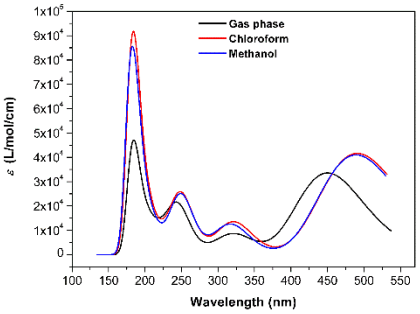




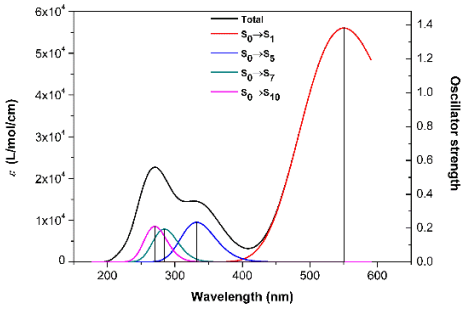
(a) Contribution of the crucial states **(b) Comparison in different media**

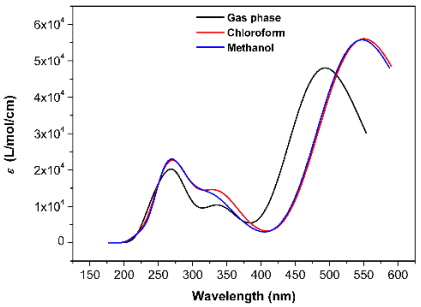
H1-1



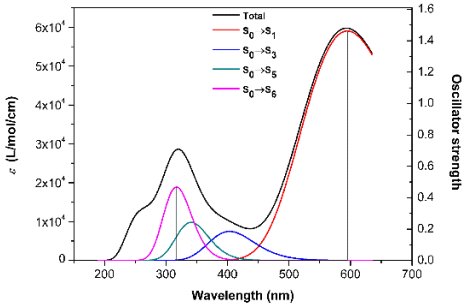


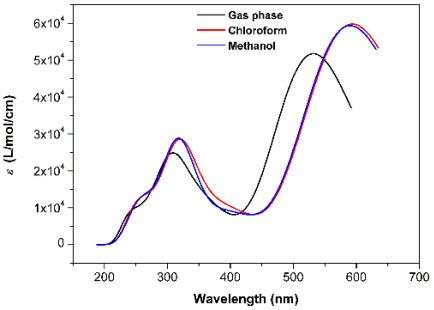
H1-2



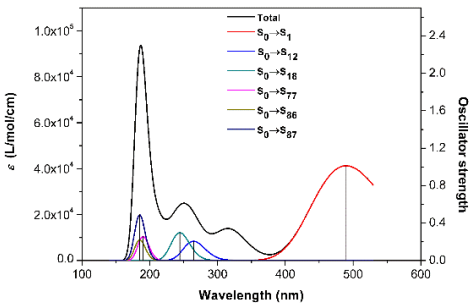


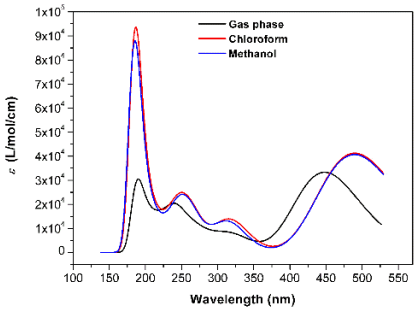
H1-3

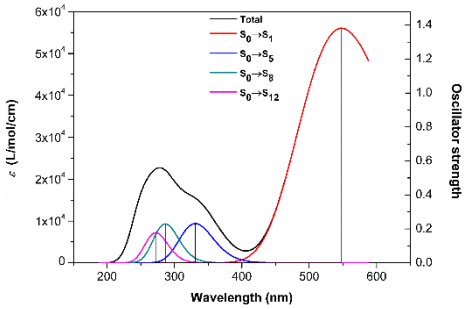
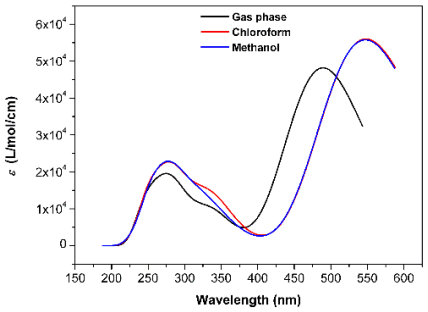
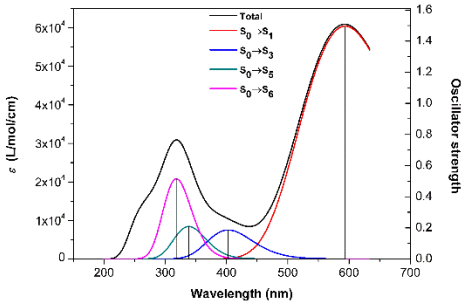
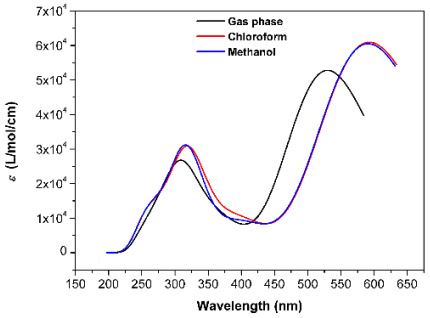
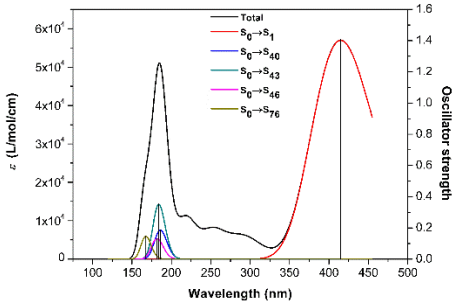
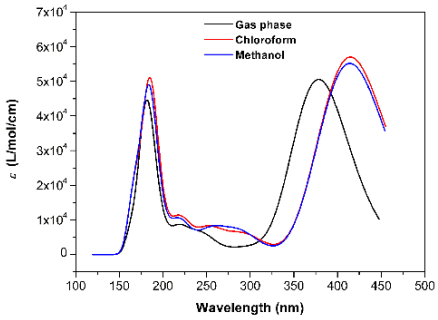
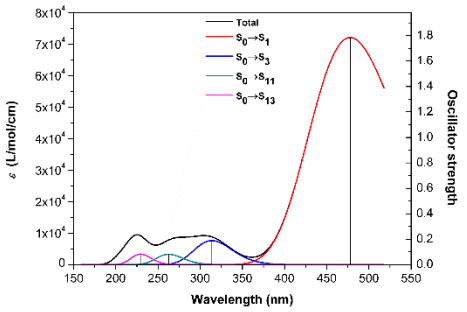
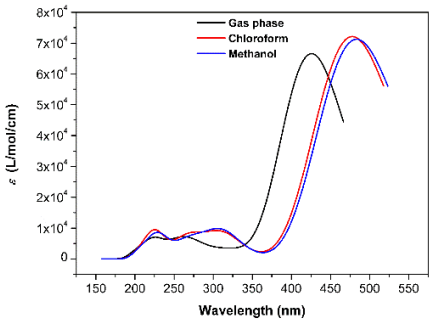




H2-1





	(a) Contribution of the crucial states	(b) Comparison in different media
H2-2		
H2-3		
B-1		
B-2		

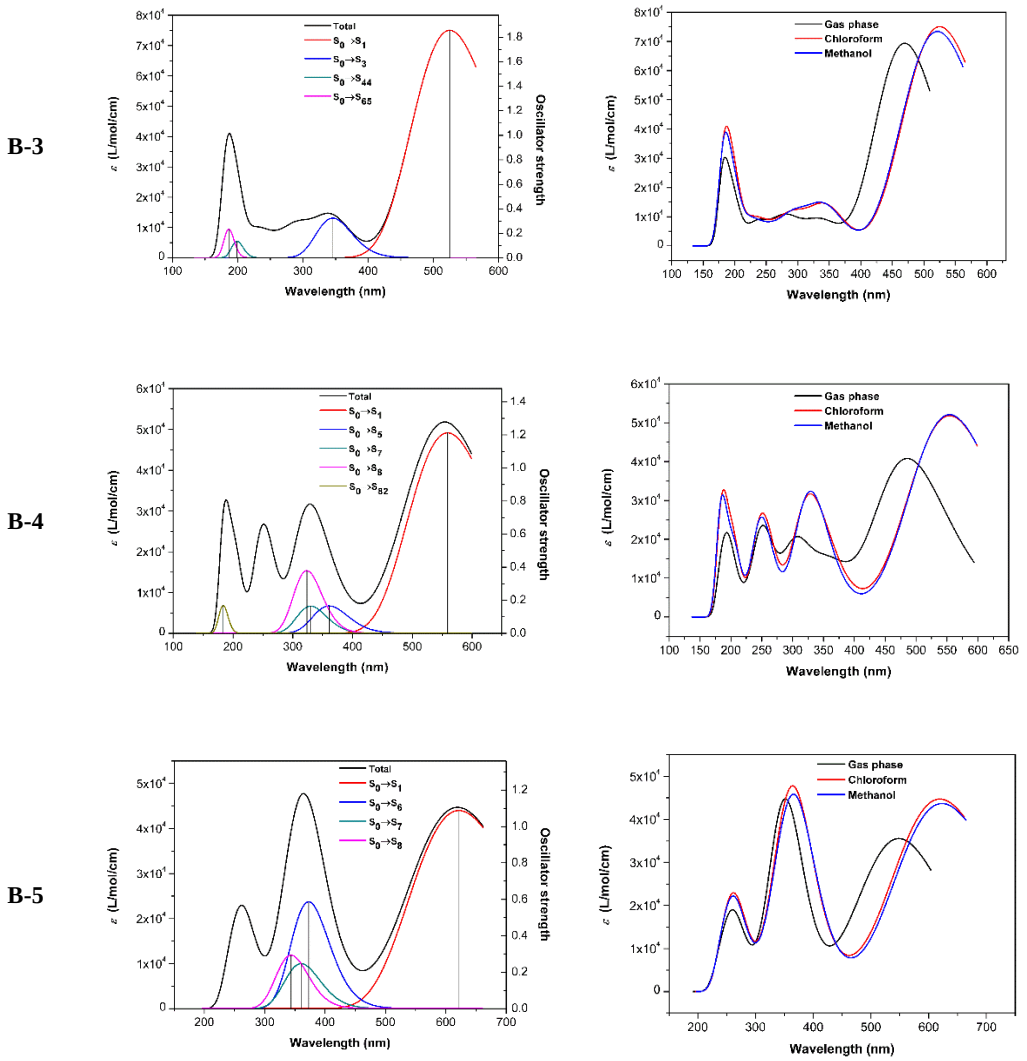
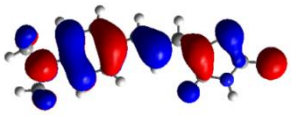
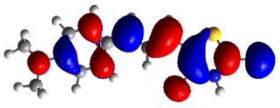
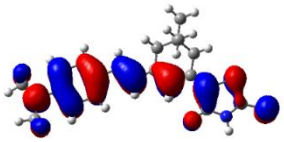
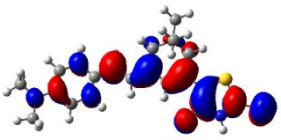
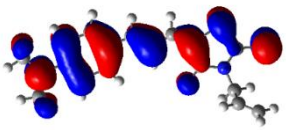
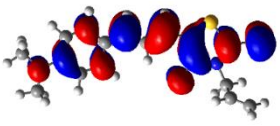
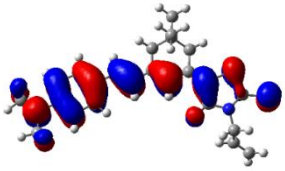
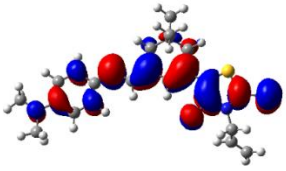
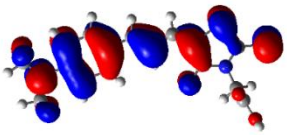
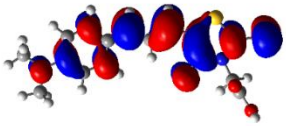
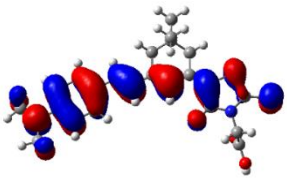
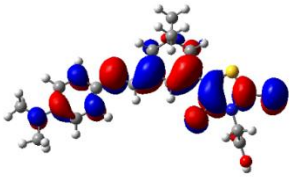
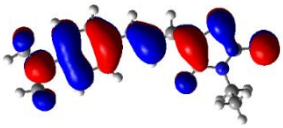
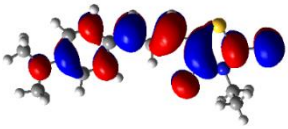
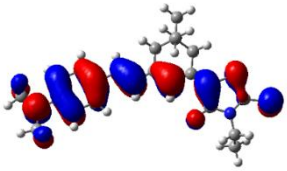
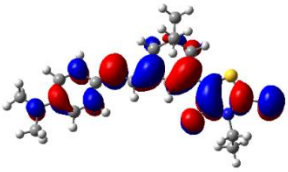
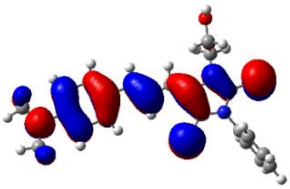
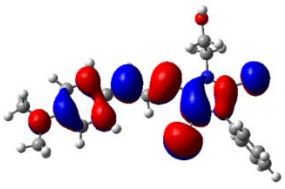


Figure S4. (a) Contribution of the crucial states to the UV-Vis spectra in chloroform, and (b) comparison of the UV-Vis spectra in different media (gas phase, chloroform, and methanol) of the R-series, H-series, and B-series.

	f	Crucial State	Excitation Assignment	Occupied Orbital	Unoccupied Orbital
R1-2	**1.636**	**S_1**	**H→L (98%)**		
R1-3	**1.798**	**S_1**	**H→L (97%)**		
R2-2	**1.663**	**S_1**	**H→L (98%)**		
R2-3	**1.827**	**S_1**	**H→L (97%)**		
R3-2	**1.651**	**S_1**	**H→L (98%)**		
R3-3	**1.809**	**S_1**	**H→L (97%)**		
R4-2	**1.651**	**S_1**	**H→L (98%)**		
R4-3	**1.816**	**S_1**	**H→L (97%)**		
H1-2	**1.385**	**S_1**	**H→L (99%)**		

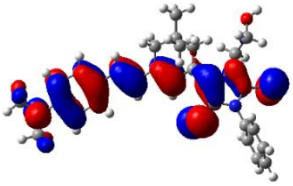
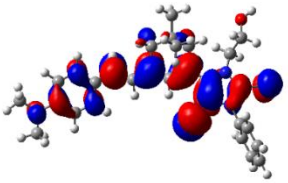
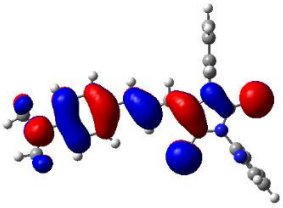
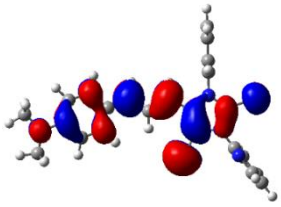
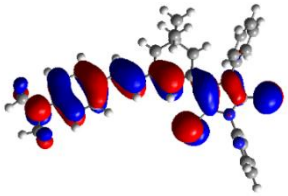
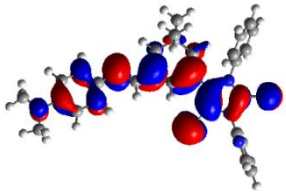
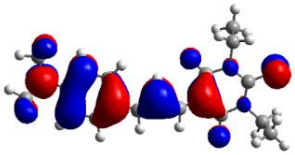
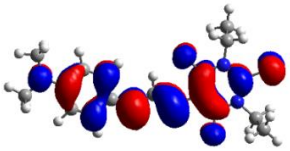
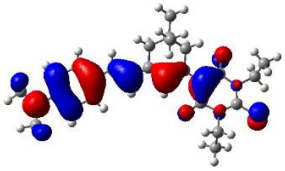
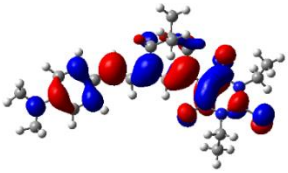
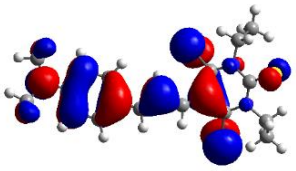
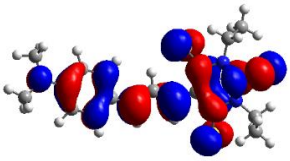
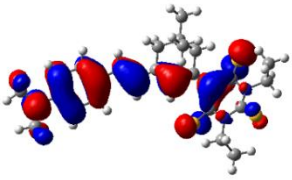
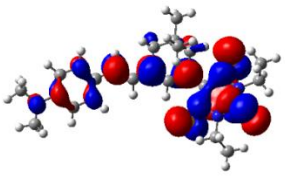
	f	Crucial State	Excitation Assignment	Occupied Orbital	Unoccupied Orbital
H1-3	**1.460**	**S_1**	**H→L (97%)**		
H2-2	**1.385**	**S_1**	**H→L (99%)**		
H2-3	**1.494**	**S_1**	**H→L (97%)**		
B-2	**1.784**	**S_1**	**H→L (97%)**		
B-3	**1.855**	**S_1**	**H→L (97%)**		
B-4	**1.215**	**S_1**	**H→L (93%)**		
B-5	**1.088**	**S_1**	**H→L (91%)**		

Fig. S5 Oscillator strengths *f* and calculated excitation assignments of the rest compounds of R-series, H-series, and B-series in chloroform at the PBE38/AUG-cc-pVDZ level. The crucial state is defined as the lowest optically allowed excited state with substantial oscillator strength in this work. H and L represent HOMO and LUMO, respectively; the percentage contributions of orbital pairs to the wave functions of excited states are given in parentheses.

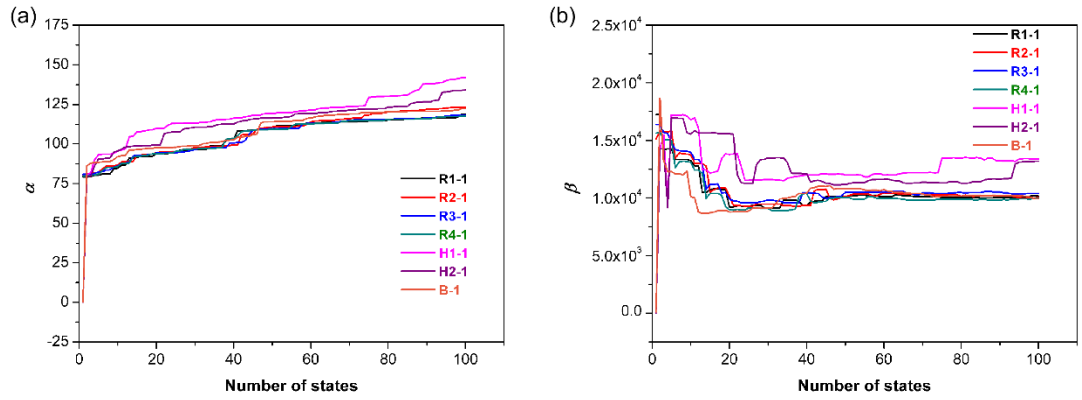


Figure S6. (a) Calculated linear polarizabilities α, and (b) molecular first-hyperpolarizabilities β according to the sum-over-states method of the representative compounds with respect to the number of excited states.

The non-covalent interactions index (NCI) analysis[4,5] was introduced to investigate the intermolecular non-covalent interactions, and the different types of non-covalent interactions can be visualized by different colors. As shown in Figure S7 below, blue indicates the strong attractive interactions, namely, hydrogen bonds, green implies the relatively weak interactions, for example, the van der Waals interaction, while red signifies the strong repulsive interactions such as steric effect. Based on this, the NCI analysis between target compounds (R1-1, H1-1, and B-1) and methanol (polar protic solvent, ε = 32.613) was carried out to study the intermolecular interactions between them, and the further investigation on the influence of such interactions on first-hyperpolarizabilities was also taken into account.

As shown in figure, in the case of R1-1, the visibly color-blocks are presented between N/O/S atoms and H atoms, therein, blue color-block appears in -N-H···O- fragment, green color-blocks present in -O-H···O- fragments and -S-H···O- fragments, which severally means the hydrogen bonds and van der Waals interactions in these fragments and verify the non-covalent interactions between target compounds and methanol. Analogously, the same conclusion can also be drawn for H1-1 and B-1.

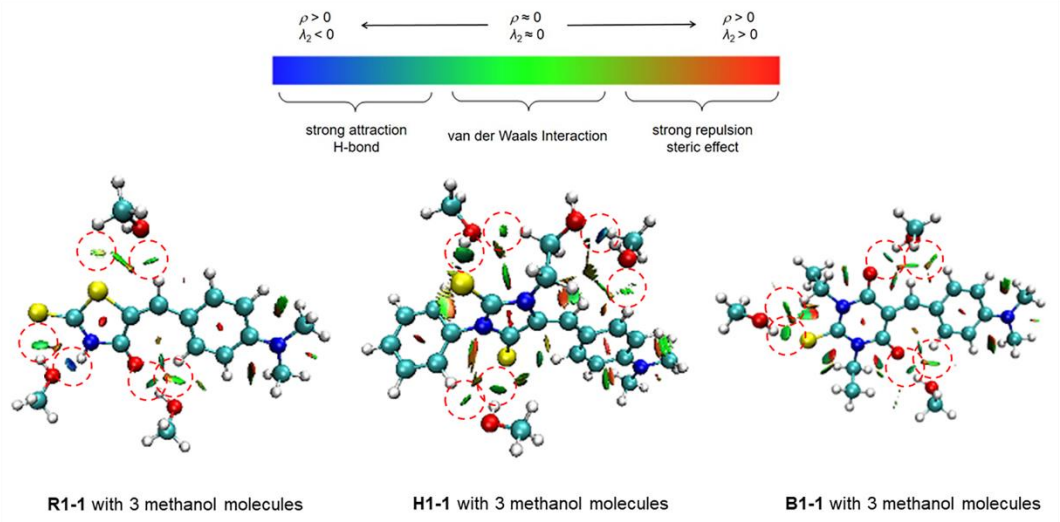


Figure S7. NCI analysis of representative compounds R1-1, H1-1, and B1-1 with three methanol.

After introducing three methanol molecules into systems, the corresponding first-hyperpolarizabilities calculated at PBE38/AUG-cc-pVDZ level and by the sum-over-states method are collected below in "with methanol" row, and the previous results without three methanol molecules are gathered in "without methanol" row, besides, the differences between them are presented in the square brackets. From Table S4 we can see, the changes of β values emerges within the acceptable range (mainly below 10 × 10^{-30} esu). Therefore, although the solvent environment of methanol slightly decreases the calculated β values, we consider that this effect can be ignorable with respect to other influencing factors such as the structural modifications and alteration of computational methods.

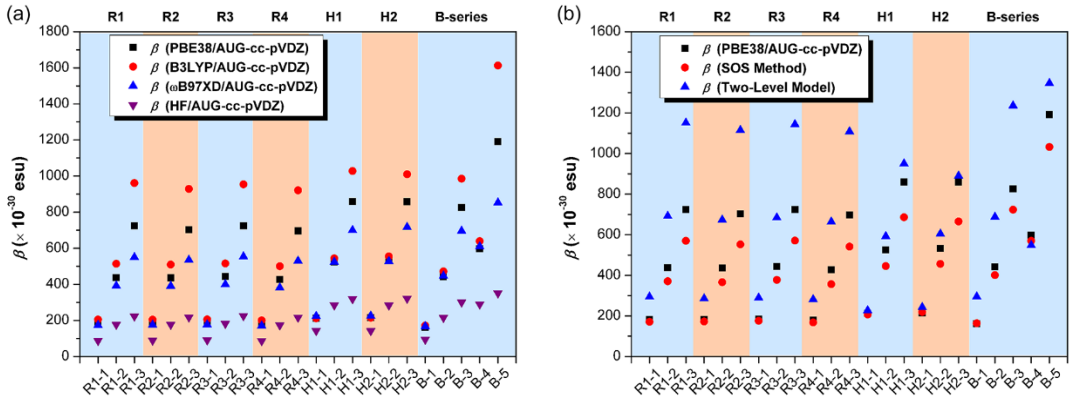


Figure S8. (a) Calculated molecular first-hyperpolarizabilities β ($\times 10^{-30}$ esu) of the R-series, H-series, and B-series in chloroform by the B3LYP, PBE38, ωB97XD, and HF functionals with AUG-cc-pVDZ basis set, and (b) calculated molecular first-hyperpolarizabilities β ($\times 10^{-30}$ esu) of the R-series, H-series, and B-series in chloroform by the PBE38 functionals with AUG-cc-pVDZ basis set, the sum-over-states method and two-level model.

Table S1. Ground state dipole moments μ_0 (Debye), HOMO and LUMO energies and their gaps (eV) of the R-series, H-series, and B-series in different media calculated at the B3LYP/6-31G** level.

	μ_0			E_{HOMO}			E_{LUMO}			E_{GAP}		
	m_1[a]	m_2[b]	m_3[c]	m_1	m_2	m_3	m_1	m_2	m_3	m_1	m_2	m_3
R1-1	9.26	12.03	14.24	-5.34	-5.18	-5.14	-2.27	-2.25	-2.25	3.07	2.93	2.89
R1-2	10.39	14.65	16.89	-5.15	-4.98	-4.97	-2.40	-2.39	-2.47	2.74	2.59	2.50
R1-3	11.07	15.71	18.13	-4.94	-4.79	-4.80	-2.41	-2.41	-2.51	2.53	2.38	2.29
R2-1	8.85	11.58	14.12	-5.27	-5.15	-5.13	-2.21	-2.22	-2.24	3.06	2.93	2.88
R2-2	9.99	14.44	16.67	-5.09	-4.96	-4.96	-2.35	-2.36	-2.45	2.74	2.59	2.51
R2-3	10.61	15.42	17.89	-4.91	-4.78	-4.80	-2.38	-2.40	-2.50	2.53	2.38	2.30
R3-1	8.79	11.47	14.00	-5.31	-5.18	-5.15	-2.24	-2.25	-2.28	3.06	2.92	2.87
R3-2	10.01	14.38	16.67	-5.12	-4.98	-4.99	-2.39	-2.39	-2.49	2.74	2.58	2.50
R3-3	10.61	15.39	17.75	-4.93	-4.80	-4.82	-2.40	-2.43	-2.53	2.52	2.37	2.28
R4-1	8.86	11.52	13.96	-5.27	-5.14	-5.12	-2.20	-2.21	-2.22	3.07	2.93	2.89
R4-2	10.01	14.38	16.54	-5.09	-4.95	-4.96	-2.34	-2.35	-2.44	2.75	2.60	2.51
R4-3	10.65	15.23	17.66	-4.89	-4.78	-4.79	-2.36	-2.39	-2.49	2.53	2.39	2.30
H1-1	7.83	11.03	14.64	-5.05	-5.02	-5.03	-2.38	-2.44	-2.48	2.68	2.58	2.54
H1-2	8.80	14.09	17.10	-4.89	-4.84	-4.85	-2.51	-2.58	-2.62	2.38	2.27	2.23
H1-3	8.50	14.01	17.01	-4.73	-4.68	-4.70	-2.53	-2.62	-2.68	2.20	2.07	2.02
H2-1	7.44	10.50	14.10	-4.98	-5.01	-5.04	-2.29	-2.43	-2.51	2.70	2.58	2.54
H2-2	8.25	13.60	16.64	-4.83	-4.84	-4.87	-2.43	-2.57	-2.64	2.40	2.28	2.23
H2-3	8.71	14.36	18.10	-4.69	-4.68	-4.72	-2.48	-2.61	-2.70	2.21	2.07	2.02
B-1	9.42	12.11	14.72	-5.61	-5.44	-5.38	-2.39	-2.36	-2.35	3.22	3.08	3.03
B-2	11.44	16.56	19.49	-5.42	-5.20	-5.22	-2.60	-2.55	-2.64	2.82	2.65	2.57
B-3	12.17	15.49	20.47	-5.16	-4.97	-4.93	-2.62	-2.62	-2.61	2.54	2.36	2.31
B-4	10.96	14.40	19.70	-5.36	-5.21	-5.19	-2.91	-2.89	-2.90	2.44	2.32	2.29
B-5	10.02	15.00	17.39	-5.03	-4.88	-4.86	-2.84	-2.88	-2.91	2.19	2.01	1.95

[a]gas phase; [b]chloroform; [c]methanol.

Table S2. Wavelengths of the absorption maxima λ_{max} (nm), oscillator strengths *f*, transition dipole moments $\Delta\mu_{eg}$ (Debye), and electronic absorption energies ΔE_{eg} (eV) of the R-series, H-series, and B-series in chloroform and methanol calculated at the PBE38/AUG-cc-pVDZ level.

	λ_{max}		*f*		ΔE_{eg}		$\Delta\mu_{eg}$	
	m_1[a]	m_2[b]	m_1	m_2	m_1	m_2	m_1	m_2
R1-1	428	427	1.247	1.205	2.88	2.91	10.65	10.46
R1-2	478	482	1.636	1.591	2.59	2.57	12.90	12.77
R1-3	514	518	1.798	1.738	2.41	2.39	14.02	13.84
R2-1	430	428	1.266	1.226	2.88	2.88	10.75	10.57
R2-2	479	483	1.663	1.617	2.59	2.57	13.01	12.89
R2-3	513	518	1.827	1.764	2.42	2.39	14.13	13.94
R3-1	430	429	1.257	1.218	2.88	2.88	10.72	10.54
R3-2	480	485	1.651	1.605	2.58	2.55	12.99	12.87
R3-3	516	521	1.809	1.746	2.41	2.38	14.09	13.91
R4-1	428	427	1.255	1.216	2.88	2.91	10.69	10.50
R4-2	477	482	1.651	1.606	2.60	2.57	12.95	12.83
R4-3	513	518	1.816	1.754	2.42	2.40	14.07	13.90
H1-1	491	490	1.004	1.004	2.53	2.53	10.24	10.22
H1-2	550	547	1.385	1.378	2.25	2.27	12.73	12.66
H1-3	594	591	1.460	1.458	2.09	2.10	13.59	13.53
H2-1	490	489	1.020	1.006	2.53	2.53	10.30	10.23
H2-2	548	547	1.385	1.379	2.26	2.27	12.70	12.66
H2-3	593	591	1.494	1.489	2.09	2.10	13.73	13.68
B-1	415	414	1.408	1.364	2.99	2.99	11.14	10.96
B-2	478	483	1.784	1.762	2.60	2.57	13.46	13.45
B-3	525	522	1.855	1.815	2.37	2.37	14.39	14.19
B-4	559	557	1.215	1.250	2.23	2.23	12.02	12.17
B-5	621	624	1.088	1.068	2.00	1.99	11.99	11.91

[a]chloroform; [b]methanol.

Table S3. Calculated maximum absorption wavelengths (λ_{max}^{cal}, nm) and first-hyperpolarizabilities β(β_{prj}^{cal}, × 10^{-30} esu) of R1-1, R3-1, R4-1, B-1, and B-2 at the PBE38/AUG-cc-pVDZ level, compared with the experimental data (λ_{max}^{exp} and β^{exp}).

	experimental data[a]		computational data		
	λ_{max}^{exp}	β^{exp}	λ_{max}^{cal}		β_{prj}^{cal}
			chloroform	methanol	chloroform
R1-1	480[1]	-	428	427	181
			[-52]	[-53]	-
	450[2]	514[2]	428	427	181
			[-22]	[-23]	[-333]
R3-1	460[2]	424[2]	430	429	183
			[-30]	[-31]	[-241]
R4-1	463[2]	477[2]	428	427	179
			[-35]	[-36]	[-298]
B-1	495[2]	116[2]	415	414	161
			[-80]	[-81]	[45]
	484[3]	68[3]	415	414	161
			[-69]	[-70]	[93]
B-2	572[3]	256[3]	478	483	438
			[-94]	[-89]	[182]

[a]Experimental data are collected from the references below for R1-1 (4 in reference [1] and 2a in reference [2]), R3-1 (2c in reference [2]), R4-1 (2b in reference [2]), B-1 (2f in reference [2] and 1[0] in reference [3]), and B-2 (1[1] in reference [3]), respectively. Differences between the calculated values and the experimental results are presented in the square brackets.

[1] H. Ikeda, Y. Kawabe, T. Sakai and K. Kawasaki, *Chem. Lett.*, 1989, 1803-1806.
[2] Q. D. Zheng, Z. G. Yao, J. Q. Cheng, Y. C. Shen, Z. H. Lu, *Chem. Lett.*, 2000, **29**, 1426-1427.
[3] S. R. Marder, L. T. Cheng, B. G. Tiemann, A. C. Friedli, M. Blanchard-Desce, J. W. Perry and J. Skindhoej, *Science*, 1994, **263**, 511-514.

Table S4. Calculated first-hyperpolarizability β ($\times 10^{-30}$ esu) of representative compounds R1-1, H1-1, and B1-1 at PBE38/AUG-cc-pVDZ level and by the sum-over-states method in situations that with or without three methanol molecules.

	β_{SOS}			β_{PBE38}		
	R1-1	H1-1	B-1	R1-1	H1-1	B-1
Without methanol	171.12	206.86	163.73	181.89	212.56	162.11
With methanol	163.60 [7.52]	191.36 [15.50]	159.24 [4.49]	182.75 [-0.86]	203.44 [9.12]	151.31 [10.80]

[4] J. Contreras-Garc á, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan and W. T. Yang, *J. Chem. Theory Comput.*, 2011, **7**, 625-632.

[5] E. R. Johnson, S. Keinan, P. Mori-S ánchez, J. Contreras-Garc á, A. J. Cohen and W. T. Yang, *J. Am. Chem. Soc.*, 2010, **132**, 6498-6506.

Table S5. Linear polarizabilities α ($\times 10^{-25}$ esu[a]) of the R-series, H-series, and B-series in different media calculated by the sum-over-states method.

	α		
	Gas phase	Chloroform	Methanol
R1-1	176.16	240.44	231.43
R1-2	229.73	312.54	309.70
R1-3	302.12	405.59	400.67
R2-1	182.50	249.56	240.87
R2-2	231.92	311.56	309.12
R2-3	306.55	407.45	401.57
R3-1	174.90	237.46	230.25
R3-2	230.51	311.11	309.35
R3-3	305.21	407.58	403.86
R4-1	174.24	237.98	230.14
R4-2	229.63	310.60	307.77
R4-3	304.13	406.33	401.40
H1-1	210.46	317.38	305.70
H1-2	265.83	373.31	364.15
H1-3	351.06	481.33	468.78
H2-1	198.88	318.57	308.22
H2-2	262.83	371.96	365.49
H2-3	353.26	490.56	480.20
B-1	181.36	246.90	238.26
B-2	237.50	325.82	328.12
B-3	344.25	466.93	450.90
B-4	307.51	443.61	434.55
B-5	342.87	480.83	471.64

[a]electrostatic unit.

Table S6. Molecular first-hyperpolarizabilities β ($\times 10^{-30}$ esu[a]) of the R-series, H-series, and B-series in different media calculated by the sum-over-sates method.

	β			β_{prj}[b]			$\beta_{\|\|}$[c]		
	m_1[d]	m_2[e]	m_3[f]	m_1	m_2	m_3	m_1	m_2	m_3
R1-1	87.98	171.12	179.02	87.94	170.84	178.68	52.77	102.50	107.21
R1-2	182.56	371.15	400.30	182.02	368.99	396.55	109.21	221.40	237.93
R1-3	297.65	569.81	617.43	281.92	539.38	577.84	169.15	323.63	346.71
R2-1	86.75	172.37	181.71	86.53	172.32	181.68	51.92	103.39	109.01
R2-2	182.76	366.10	400.76	182.70	365.92	400.13	109.62	219.55	240.08
R2-3	284.21	552.46	611.95	275.81	533.76	586.60	165.49	320.26	351.96
R3-1	89.79	176.01	186.34	88.53	174.52	184.92	53.12	104.71	110.95
R3-2	187.25	377.59	412.76	186.21	376.02	410.63	111.73	225.61	246.38
R3-3	293.92	571.39	634.44	286.75	555.56	613.55	172.05	333.34	368.13
R4-1	85.98	168.08	176.62	85.62	167.95	176.55	51.37	100.77	105.93
R4-2	177.49	356.48	387.40	177.40	356.34	386.75	106.44	213.81	232.05
R4-3	280.32	541.93	594.02	272.92	526.22	571.30	163.75	315.73	342.78
H1-1	115.74	206.86	214.88	113.60	204.32	212.05	68.16	122.59	127.23
H1-2	227.52	445.40	460.50	224.37	439.10	451.13	134.62	263.46	270.68
H1-3	356.04	686.40	716.56	323.30	606.98	619.94	193.98	364.19	371.97
H2-1	113.96	219.28	234.36	111.80	215.61	229.90	67.08	129.37	137.94
H2-2	218.57	456.46	486.62	215.20	446.66	473.27	129.12	267.99	283.96
H2-3	307.61	665.87	723.34	279.40	593.62	633.08	167.64	356.17	379.85
B-1	85.78	163.73	171.42	82.87	160.42	168.30	49.72	96.25	100.98
B-2	202.42	401.01	437.22	196.66	392.93	429.64	117.99	235.76	257.78
B-3	395.74	723.77	733.71	360.07	668.45	677.56	216.04	401.07	406.53
B-4	301.53	570.17	596.99	300.29	567.60	594.06	180.18	340.56	356.44
B-5	538.69	1032.43	1077.51	523.72	1001.20	1041.03	314.23	600.72	624.62

[a]electrostatic unit; [b]β calculated along the molecular dipole direction; [c]parallel component of the β_{prj} ($\beta_{||} = 3/5\,\beta_{prj}$); [d]gas phase; [e]chloroform; [f]methanol.

Table S7. Molecular first-hyperpolarizabilities β ($\times 10^{-30}$ esu[a]) of the R-series, H-series, and B-series in chloroform calculated by the functionals PBE38, B3LYP, ωB97XD, and HF with AUG-cc-pVDZ basis set.

	PBE38			B3LYP			ωB97XD			HF		
	β	β_{prj}[b]	$\beta_{\|\|}$[c]	β	β_{prj}	$\beta_{\|\|}$	β	β_{prj}	$\beta_{\|\|}$	β	β_{prj}	$\beta_{\|\|}$
R1-1	181.89	181.45	108.87	205.24	204.75	122.85	173.62	173.28	103.97	87.45	86.31	51.78
R1-2	437.76	435.02	261.01	514.54	511.54	306.92	392.15	390.08	234.05	176.83	172.48	103.49
R1-3	724.27	692.96	415.77	960.96	923.26	553.96	550.28	527.30	316.38	222.88	200.91	120.55
R2-1	182.83	182.82	109.69	204.47	204.46	122.68	175.30	175.27	105.16	88.90	88.60	53.16
R2-2	436.07	435.71	261.43	509.78	509.40	305.64	391.08	390.92	234.55	176.94	175.13	105.08
R2-3	702.97	684.58	410.75	928.76	906.93	544.16	535.53	522.77	313.66	217.14	201.65	120.99
R3-1	184.26	182.96	109.78	205.62	204.29	122.57	177.29	175.85	105.51	90.68	89.81	53.88
R3-2	443.87	442.07	265.24	516.11	514.25	308.55	400.32	398.43	239.06	181.92	179.88	107.93
R3-3	724.30	708.89	425.33	954.07	935.94	561.57	554.12	543.40	326.04	224.66	210.43	126.26
R4-1	178.59	178.54	107.13	200.38	200.34	120.20	170.75	170.67	102.40	86.61	86.38	51.83
R4-2	426.85	426.69	256.01	500.61	500.44	300.26	382.18	382.12	229.27	173.21	171.73	103.04
R4-3	696.70	680.93	408.56	921.41	902.70	541.62	530.12	519.28	311.57	216.15	201.80	121.08
H1-1	212.56	210.11	126.07	212.30	210.08	126.05	224.31	221.60	132.96	142.39	140.42	84.25
H1-2	524.70	517.35	310.41	544.25	537.27	322.36	524.41	517.36	310.42	284.61	279.22	167.53
H1-3	858.91	786.75	472.05	1027.72	948.54	569.12	700.52	643.25	385.95	318.77	277.54	166.53
H2-1	214.89	210.85	126.51	215.49	211.74	127.05	225.61	221.09	132.65	142.04	138.72	83.23
H2-2	532.24	520.40	312.24	555.44	543.92	326.35	528.08	516.44	309.86	283.97	275.60	165.36
H2-3	858.73	789.55	473.73	1010.28	934.92	560.95	717.28	661.35	396.81	321.40	279.64	167.78
B-1	162.11	160.60	96.36	171.62	170.13	102.08	167.98	166.64	99.98	93.92	91.70	55.02
B-2	442.09	437.71	262.63	472.04	467.86	280.71	447.05	443.23	265.94	215.08	207.84	124.71
B-3	826.24	781.45	468.87	985.29	939.34	563.60	696.10	657.36	394.41	300.53	263.11	157.86
B-4	597.52	595.71	357.43	639.56	638.10	382.86	610.12	608.38	365.03	289.54	284.65	170.79
B-5	1191.24	1163.17	697.90	1612.75	1583.53	950.12	852.76	830.76	498.46	351.33	327.29	196.37

[a]electrostatic unit; [b]β calculated along the molecular dipole direction; [c]parallel component of the β_{prj} ($\beta_{||} = 3/5\,\beta_{prj}$).