Supporting information

Investigation of a benzodiazaborine library to identify new pH-responsive fluorophore

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Contents

1. Results of primary screening for UV–Vis and fluorescence spectral measurement of starting materials (A-N, 1-17)

o-Formylphenylboronic acids (A-N):

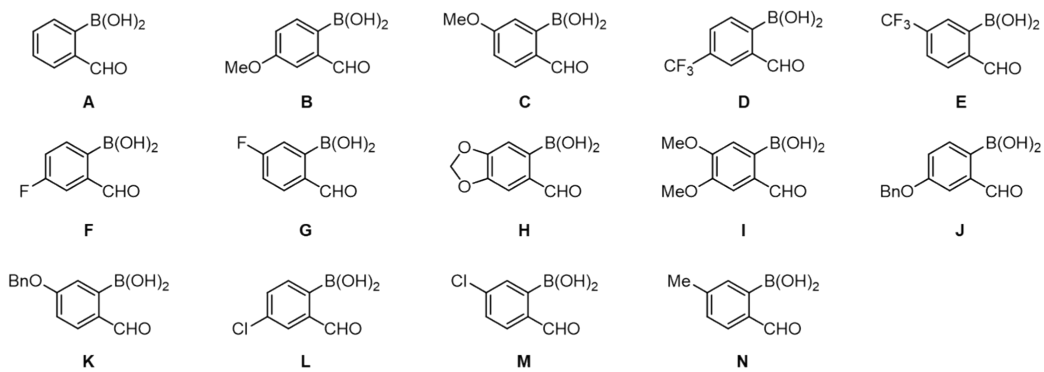


Figure S1. Structure of *o*-formylphenylboronic acids (**A-N**) used to construct a bDAB library.

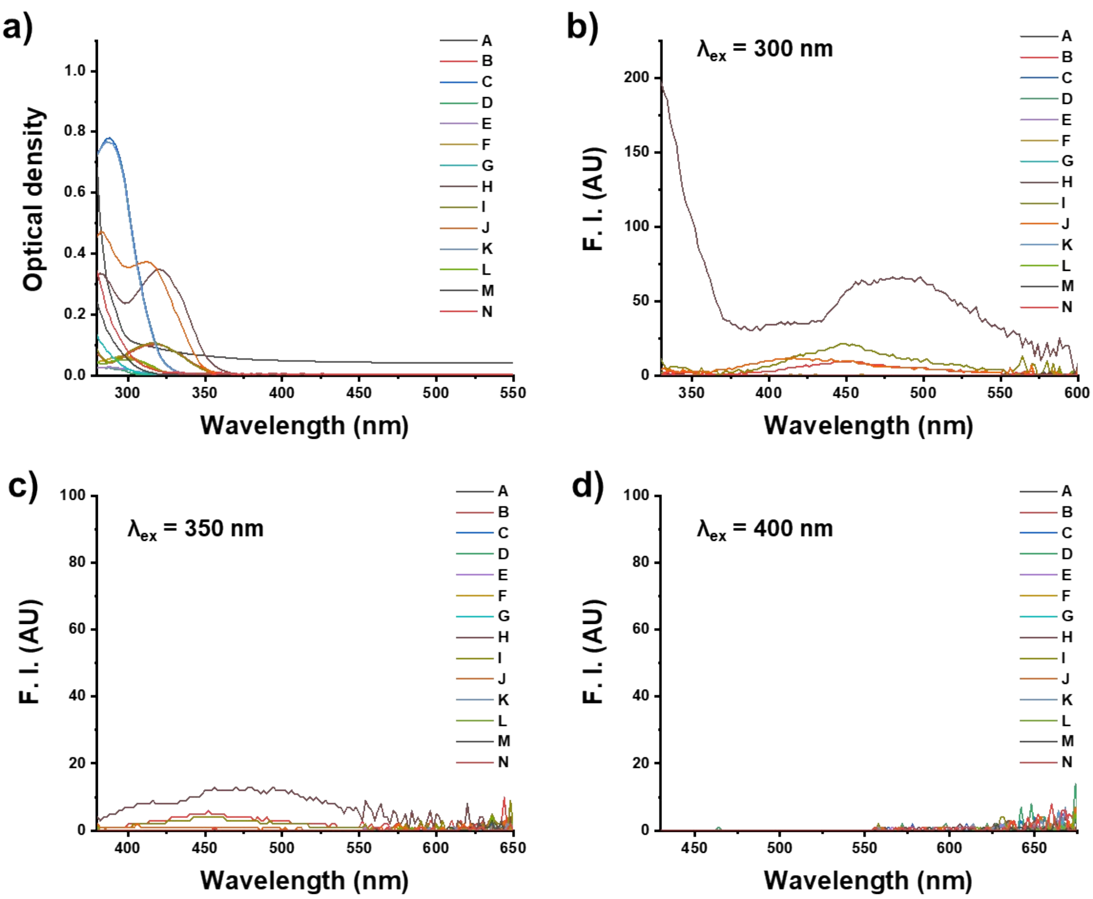


Figure S2. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective *o*-formylphenylboronic acids (**A**-**N**) at pH 4.0, [**A**-**N**] = 100 μM in 20 mM citrate buffer with 10% DMSO.

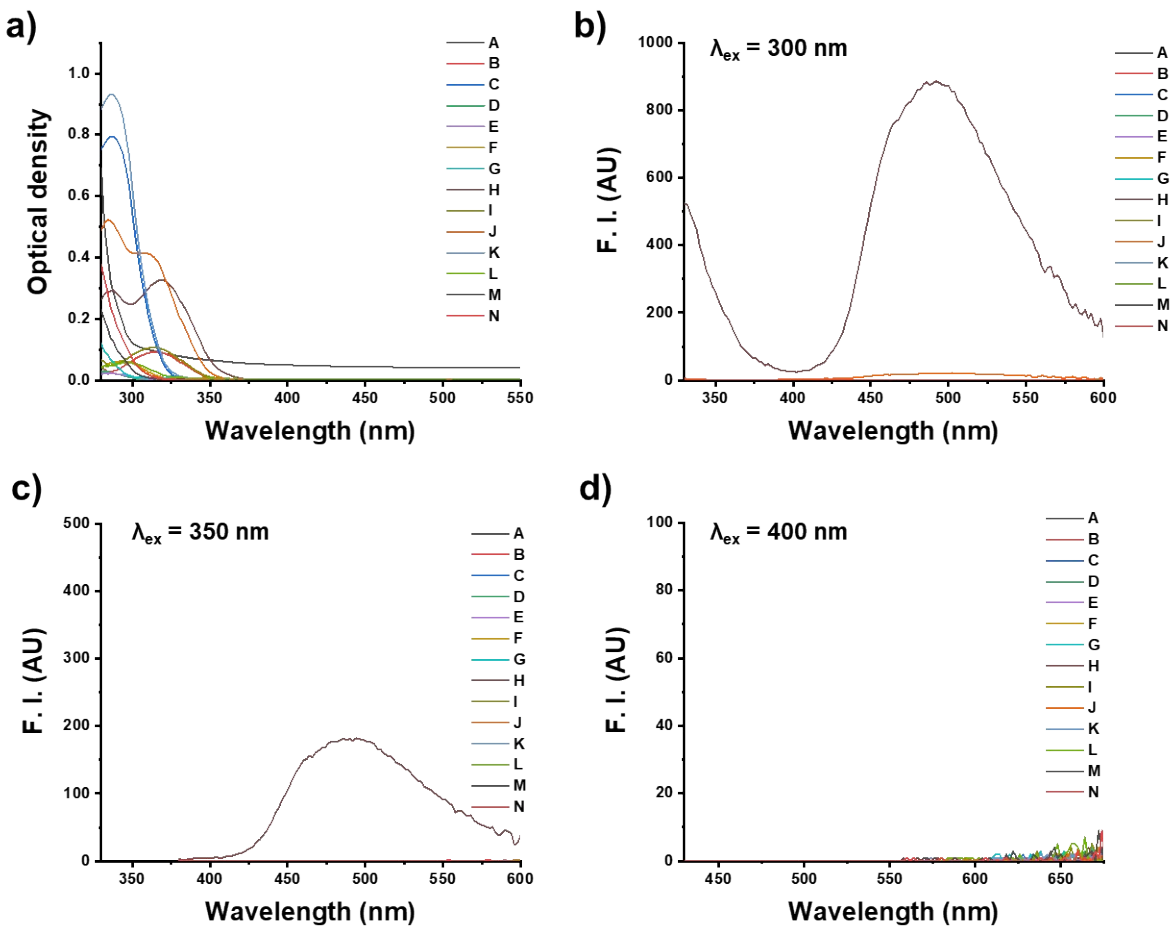


Figure S3. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective *o*-formylphenylboronic acids (**A**-**N**) at pH 6.0, [**A**-**N**] = 100 μM in 20 mM phosphate buffer with 10% DMSO.

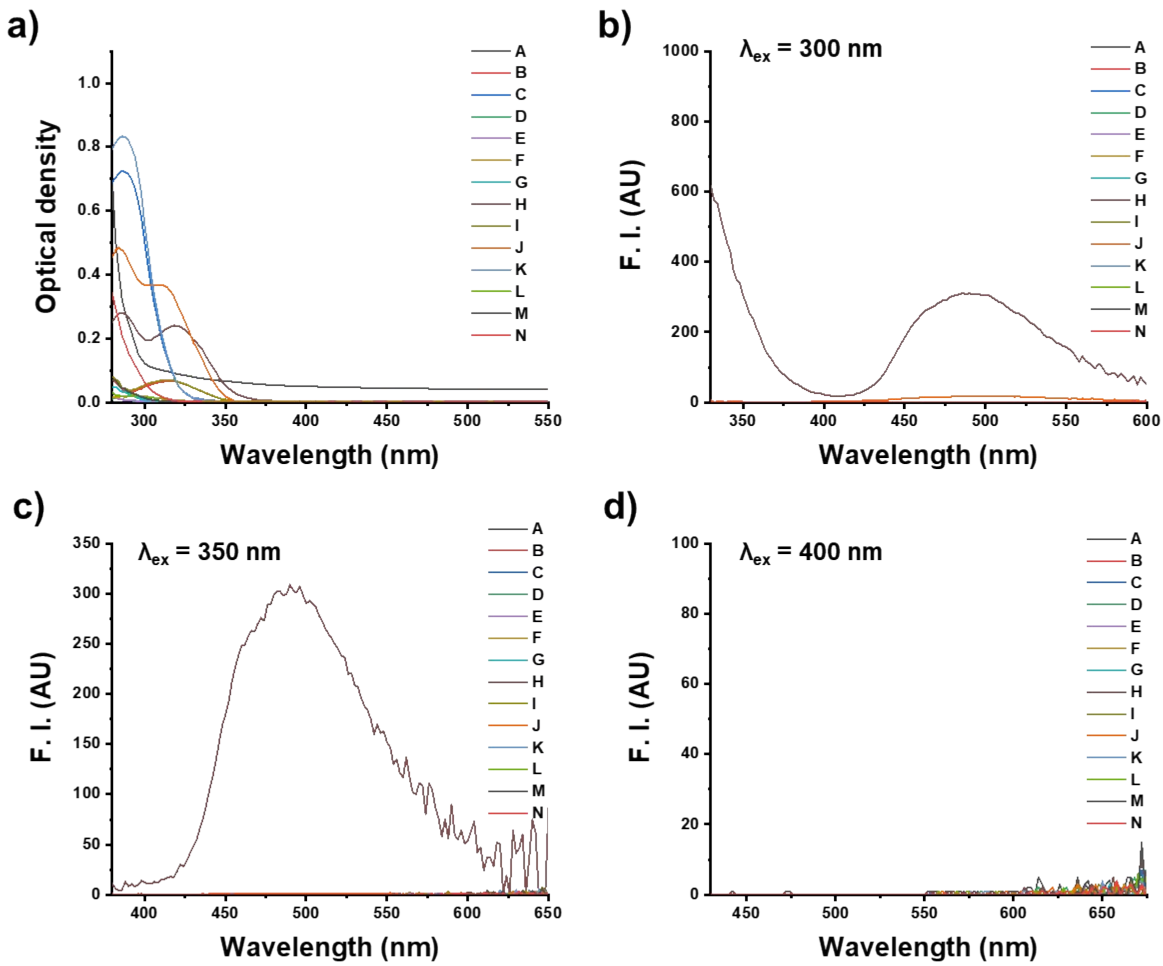


Figure S4. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective *o*-formylphenylboronic acids (**A**-**N**) at pH 7.0, [**A**-**N**] = 100 μM in 20 mM phosphate buffer with 10% DMSO.

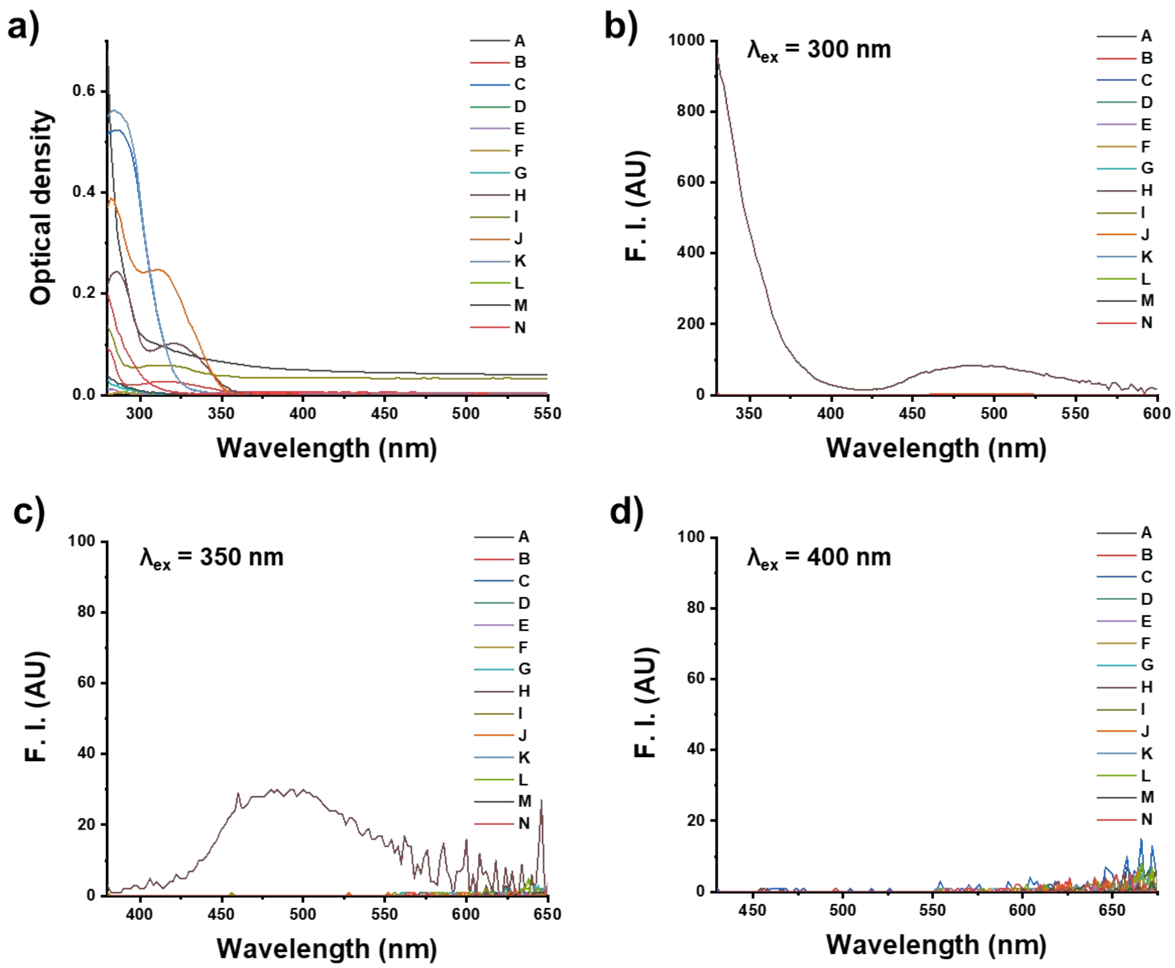


Figure S5. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective *o*-formylphenylboronic acids (**A**-**N**) at pH 8.0, [**A**-**N**] = 100 μM in 20 mM phosphate buffer with 10% DMSO.

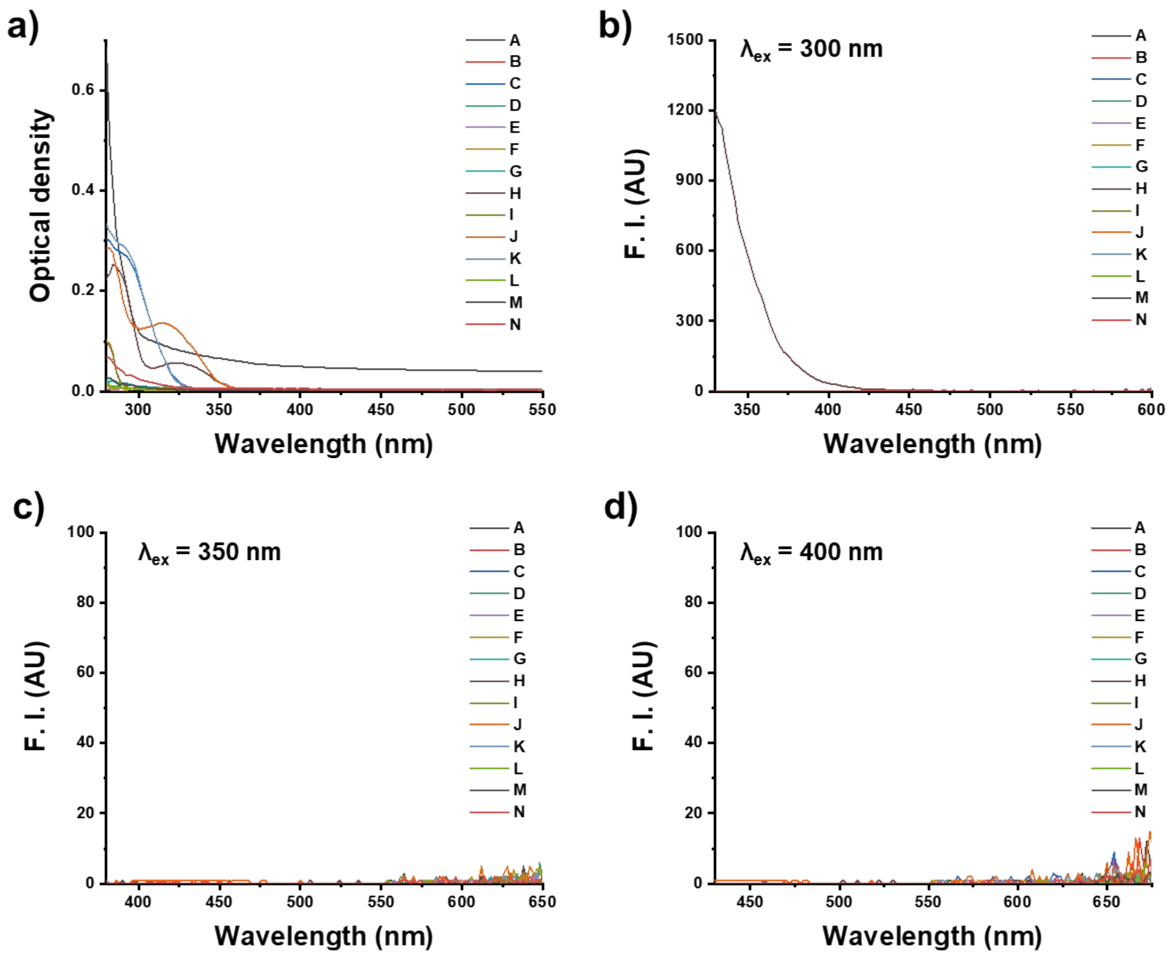


Figure S6. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective *o*-formylphenylboronic acids (**A**-**N**) at pH 10.0, [**A**-**N**] = 100 µM in 20 mM carbonate buffer with 10% DMSO.

Phenylhydrazines (1-17):

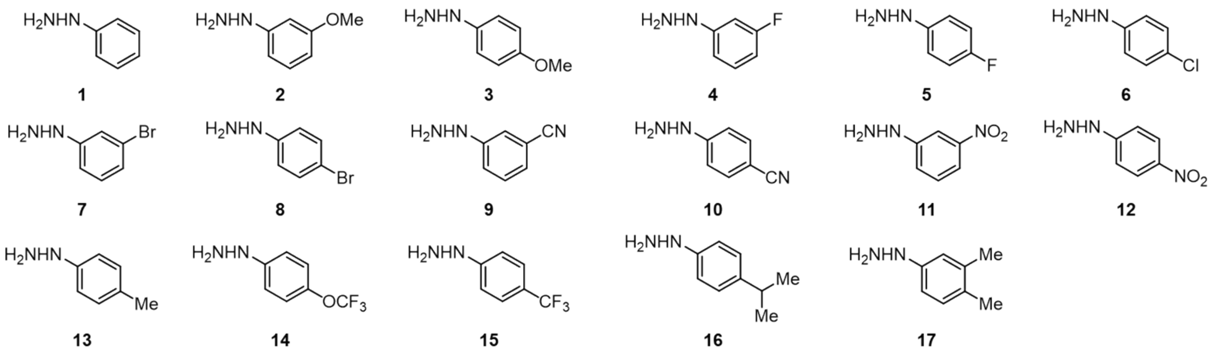


Figure S7. Structure of phenylhydrazines (**1**-**17**) used to construct a bDAB library.

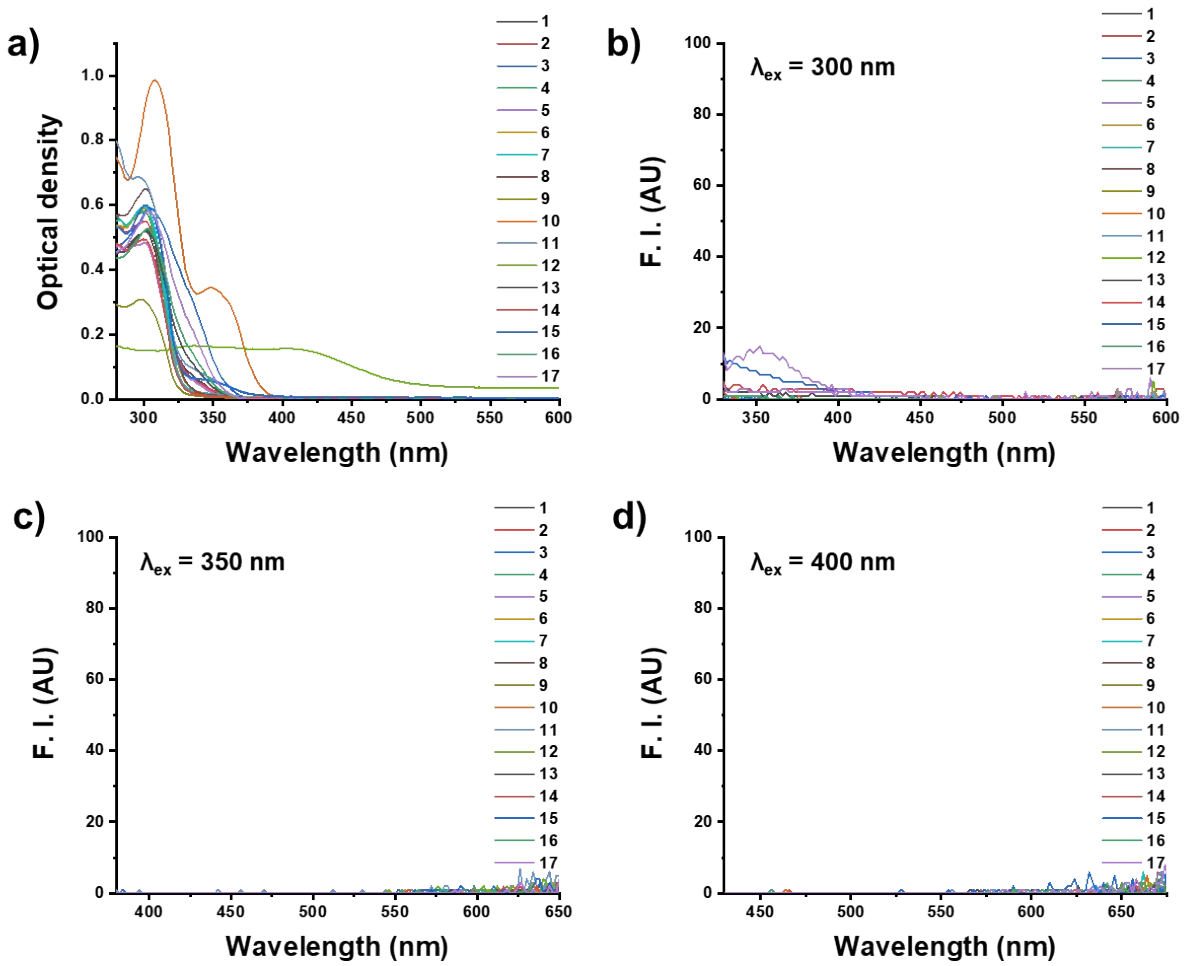


Figure S8. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective phenylhydrazines (**1**-**17**) at pH 4.0, [**1**-**17**] = 100 μM in 20 mM citrate buffer with 10% DMSO.

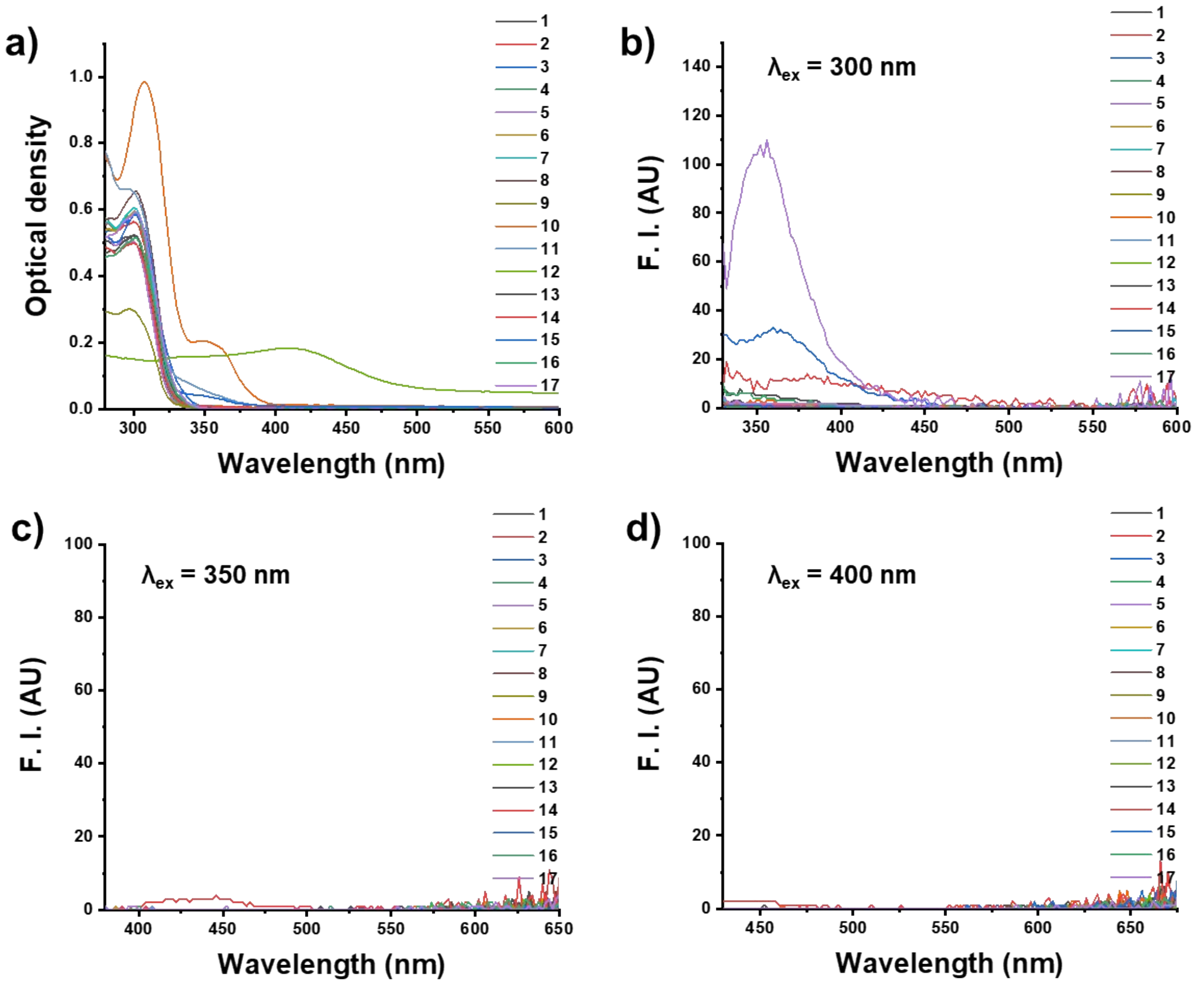


Figure S9. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective phenylhydrazines (**1**-**17**) at pH 6.0, [**1**-**17**] = 100 μM in 20 mM phosphate buffer with 10% DMSO.

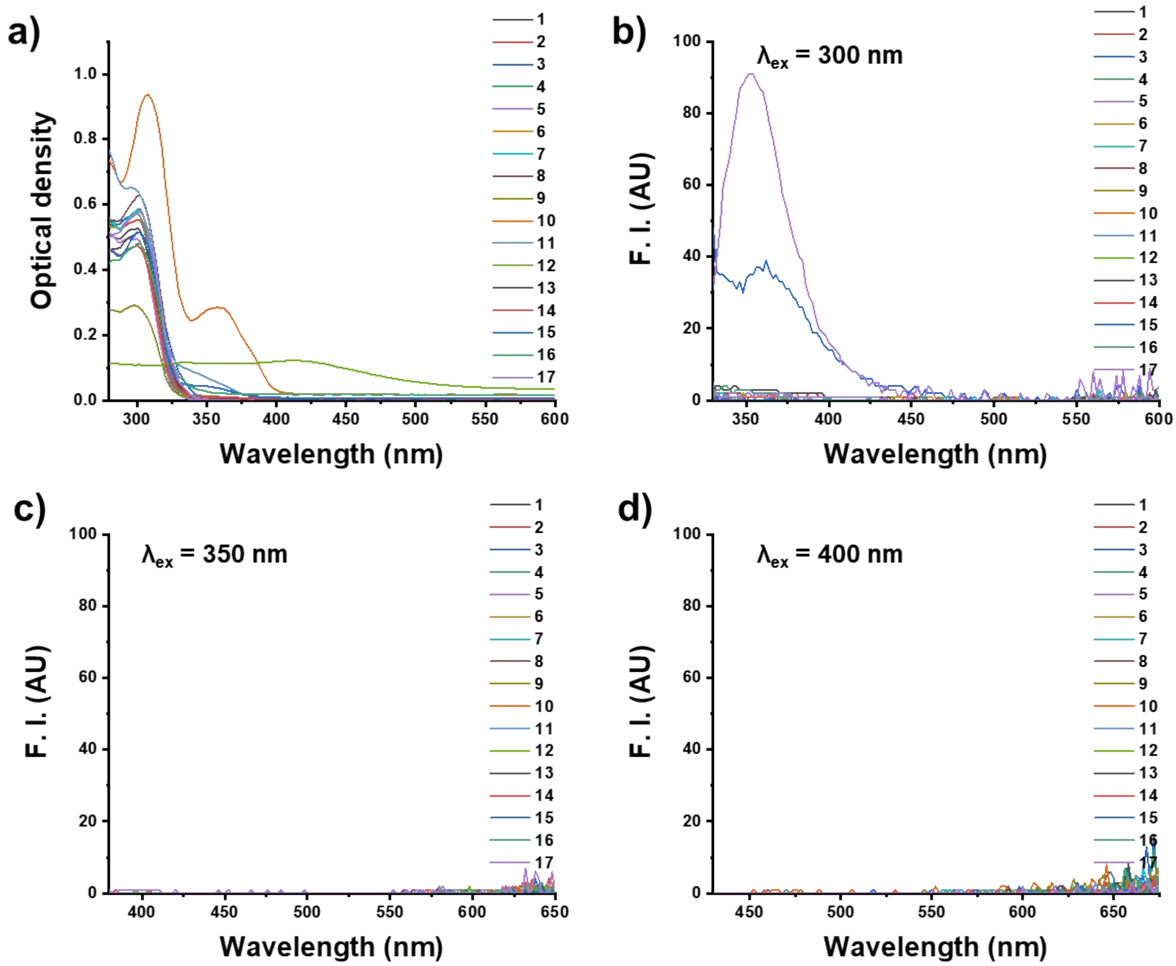


Figure S10. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective phenylhydrazines (**1**-**17**) at pH 7.0, [**1**-**17**] = 100 μM in 20 mM phosphate buffer with 10% DMSO.

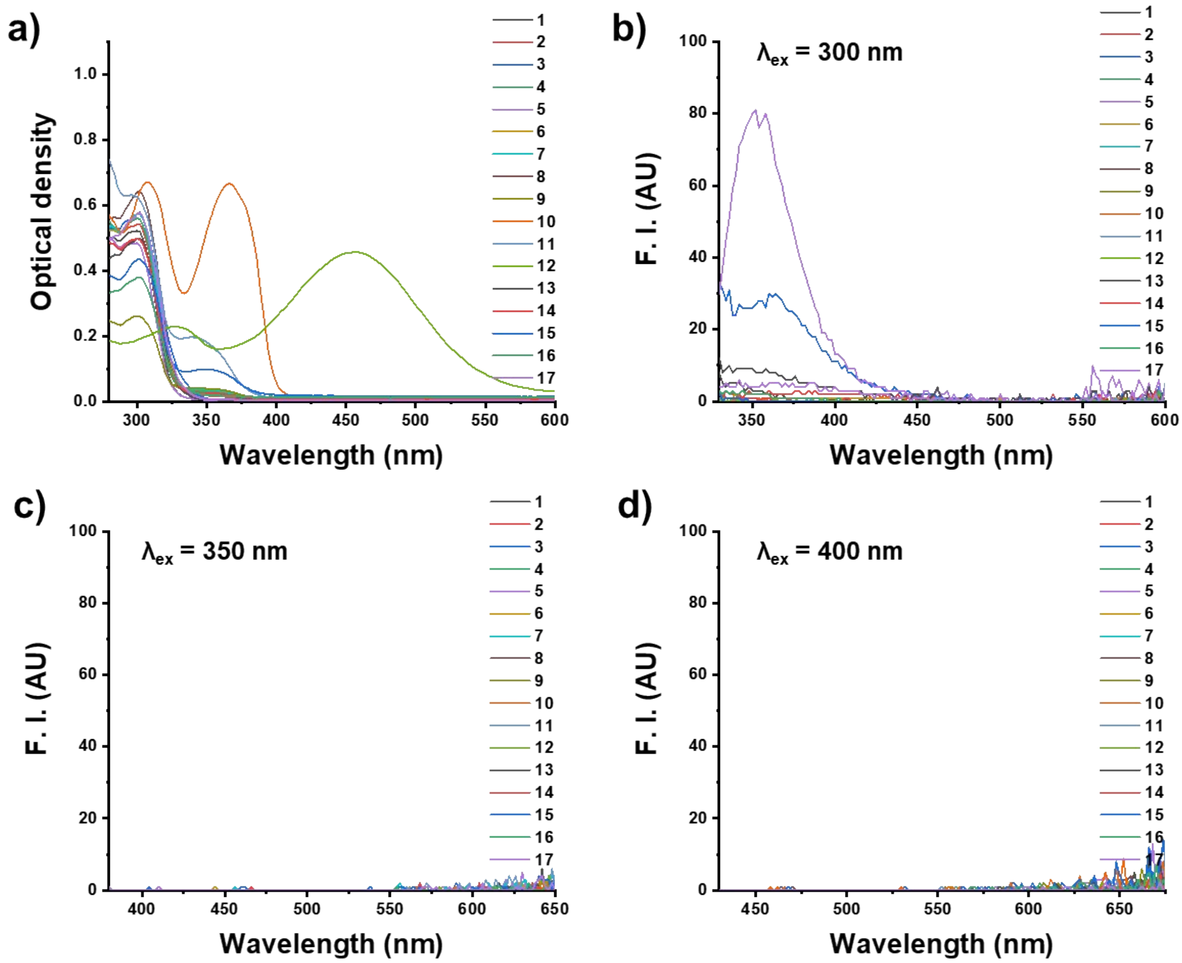


Figure S11. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective phenylhydrazines (**1-17**) at pH 8.0, [**1-17**] = 100 μM in 20 mM phosphate buffer with 10% DMSO.

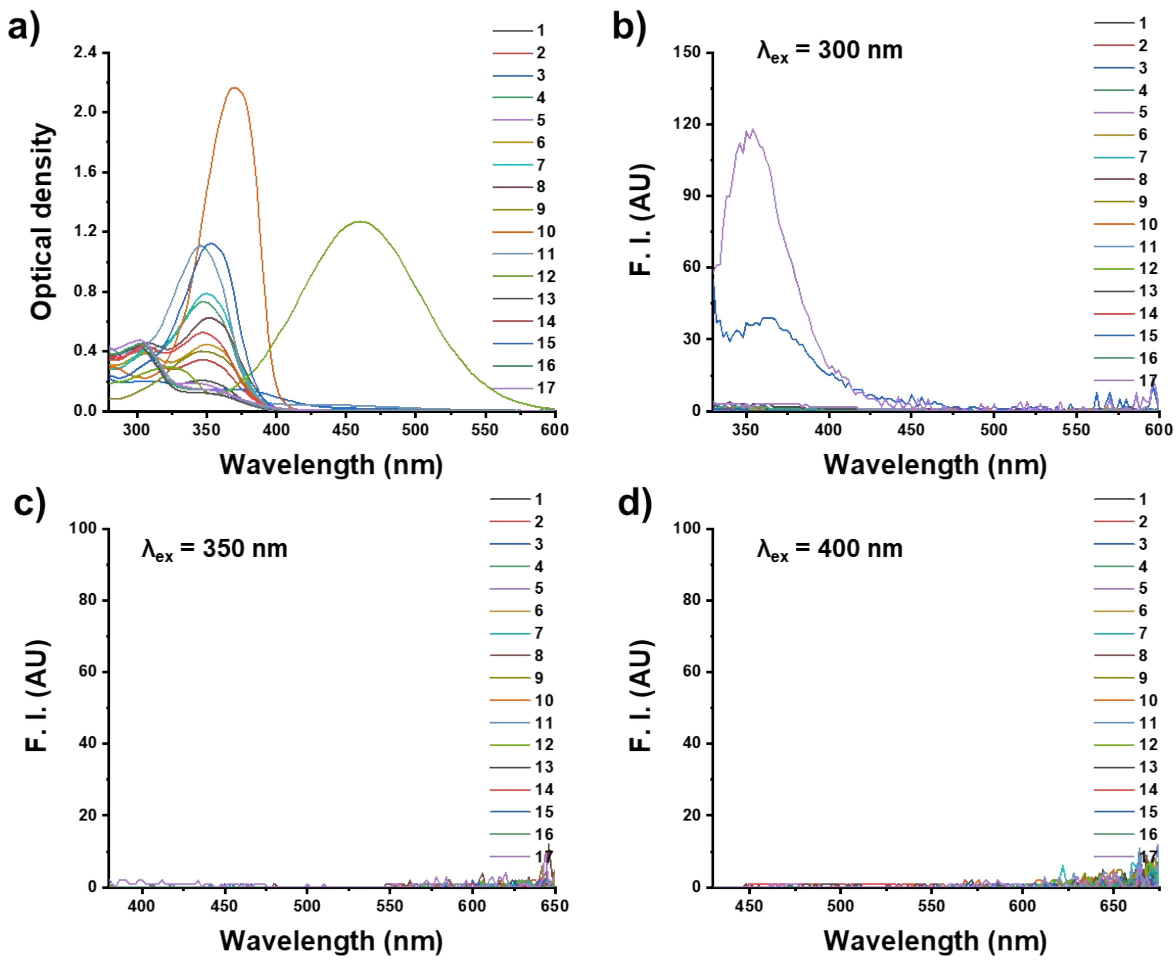


Figure S12. a) UV–Vis spectra and b), c), d) fluorescence spectra of respective phenylhydrazines (**1**-**17**) at pH 10.0, [**1**-**17**] = 100 μM in 20 mM carbonate buffer with 10% DMSO.

2. Results of primary screening for UV–Vis absorption of a bDAB library (A1-N17) under varied pH conditions

Table S1. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**A1**-**A17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
A1	300	300	300	300	300
A2	300	300	300	300	300
A3	300	300	300	300	350
A4	300	300	300	300	350
A5	300	300	300	300	300
A6	300	300	300	300	350
A7	300	300	300	300	350
A8	300	300	300	300	350
A9	300	300	300	300	350
A10	310	310	305	365	365
A11	300	300	300	300	340
A12	400	410	410	450	460
A13	300	300	300	300	300
A14	300	300	300	300	350
A15	300	300	300	300	350
A16	300	300	300	300	350
A17	300	300	300	300	300

Table S2. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**B1**-**B17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
B1	310	285	285	285	315
B2	285	285	285	285	315
B3	315	285	285	285	315
B4	285	285	285	285	350
B5	315	285	285	285	315
B6	285	285	285	285	315
B7	285	285	285	285	350
B8	285	285	285	285	315
B9	285	285	285	285	350
B10	285	285	285	285	370
B11	280	285	285	285	350
B12	335	335	335	335	460
B13	310	285	285	285	315

B14	285	285	285	285	315
B15	280	285	285	285	350
B16	315	315	315	315	315
B17	315	285	285	285	315

Table S3. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**C1**-**C17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
C1	340	285	285	285	285
C2	285	285	285	285	285
C3	340	285	285	285	290
C4	285	285	285	285	345
C5	285	285	285	285	285
C6	285	285	285	285	285
C7	285	285	285	285	350
C8	285	285	285	285	350
C9	285	285	285	285	340
C10	285	285	285	365	365
C11	285	285	285	285	345
C12	285	285	285	465	470
C13	285	285	285	285	285
C14	285	285	285	285	285
C15	285	285	285	285	350
C16	340	315	325	330	285
C17	340	285	285	285	285

Table S4. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**D1**-**D17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
D1	310	310	315	315	350
D2	310	310	315	315	350
D3	310	310	315	315	320
D4	310	310	315	315	350
D5	310	310	315	315	350
D6	310	310	315	315	350
D7	310	310	315	315	360
D8	310	310	315	315	360
D9	310	310	315	350	350
D10	350	310	370	370	365

D11	285	285	285	350	350
D12	415	415	445	455	430
D13	310	310	315	315	350
D14	310	310	315	315	350
D15	310	310	315	350	350
D16	310	310	315	315	350
D17	310	285	285	315	350

Table S5. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**E1**-**E17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
E1	310	310	310	310	365
E2	310	310	310	310	365
E3	310	310	310	310	315
E4	310	310	310	310	365
E5	310	310	310	310	365
E6	310	310	310	310	365
E7	310	310	310	310	365
E8	310	310	310	310	365
E9	310	310	310	365	365
E10	355	310	370	375	370
E11	310	310	310	360	360
E12	415	415	445	450	435
E13	310	310	310	310	365
E14	310	310	310	310	365
E15	310	310	310	360	360
E16	310	310	310	310	365
E17	310	310	310	310	365

Table S6. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**F1**-**F17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
F1	300	300	300	300	300
F2	300	300	300	300	350
F3	310	300	300	300	315
F4	300	300	300	300	350
F5	300	300	300	300	305
F6	300	300	300	300	355
F7	300	300	300	300	350

F8	300	300	300	300	355
F9	300	300	300	300	355
F10	310	310	310	310	370
F11	285	285	285	285	350
F12	340	410	410	445	450
F13	300	300	300	300	305
F14	300	300	300	300	350
F15	300	300	300	300	350
F16	300	300	300	300	305
F17	300	300	300	300	305

Table S7. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**G1**-**G17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
G1	285	285	285	285	340
G2	285	285	285	285	340
G3	315	315	315	315	320
G4	285	285	285	285	345
G5	285	285	285	285	345
G6	285	285	285	285	345
G7	285	285	285	285	345
G8	285	300	300	300	345
G9	285	285	285	300	340
G10	310	310	315	365	365
G11	285	285	285	340	340
G12	420	415	455	460	450
G13	285	285	285	285	345
G14	285	285	285	285	345
G15	285	285	285	300	345
G16	285	285	285	285	345
G17	285	285	285	285	345

Table S8. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**H1**-**H17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
H1	350	300	300	300	290
H2	350	300	300	300	290
H3	350	300	300	300	355
H4	300	300	300	300	290

H5	350	300	300	300	290
H6	300	300	300	300	290
H7	300	300	300	300	290
H8	300	300	300	300	290
H9	300	300	290	300	290
H10	300	300	300	300	370
H11	285	285	285	300	350
H12	360	365	360	360	470
H13	350	300	300	300	20
H14	300	300	300	300	260
H15	300	300	300	300	355
H16	350	300	300	300	290
H17	350	300	300	300	290

Table S9. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**I1-I17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
I1	340	290	290	290	290
I2	290	290	290	290	290
I3	345	290	290	290	290
I4	290	290	290	290	290
I5	290	290	290	290	290
I6	290	290	290	290	290
I7	290	290	290	290	290
I8	290	290	290	290	290
I9	290	290	290	290	290
I10	290	300	290	295	370
I11	290	290	290	290	345
I12	355	355	360	365	470
I13	340	290	290	290	290
I14	290	290	290	290	290
I15	340	290	290	290	355
I16	340	290	300	290	290
I17	340	290	290	290	290

Table S10. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**J1-J17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
J1	320	320	310	315	330

J2	315	310	310	315	315
J3	320	310	310	315	315
J4	310	310	310	315	315
J5	315	310	310	315	315
J6	320	310	310	315	325
J7	315	310	310	315	325
J8	330	310	310	315	325
J9	305	310	310	315	315
J10	315	310	315	315	355
J11	285	285	285	285	315
J12	330	330	330	330	465
J13	315	310	310	315	315
J14	320	310	310	315	315
J15	315	310	310	315	350
J16	325	310	310	315	315
J17	320	310	310	315	325

Table S11. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**K1**-**K17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
K1	335	295	295	295	295
K2	335	295	295	295	295
K3	340	295	295	295	295
K4	295	295	295	295	295
K5	295	295	295	295	295
K6	295	295	295	295	295
K7	295	295	295	295	330
K8	335	295	295	295	295
K9	295	295	295	295	340
K10	330	295	295	295	370
K11	295	295	295	295	340
K12	380	380	400	405	465
K13	335	295	295	295	295
K14	295	295	295	295	295
K15	295	295	295	295	350
K16	340	295	295	295	365
K17	340	295	295	295	295

Table S12. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**L1**-**L17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
L1	295	310	310	310	355
L2	295	310	310	310	355
L3	295	310	310	310	355
L4	295	310	310	310	355
L5	295	310	310	310	355
L6	295	310	310	310	355
L7	295	310	310	310	355
L8	320	310	310	330	355
L9	310	310	310	310	355
L10	295	310	310	310	370
L11	310	310	310	310	350
L12	340	345	345	455	450
L13	295	310	310	310	310
L14	295	310	310	310	355
L15	310	310	310	310	355
L16	315	310	310	310	340
L17	310	310	310	310	310

Table S13. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**M1**-**M17**).

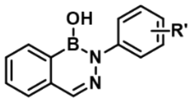
	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
M1	300	285	300	300	355
M2	300	285	285	285	355
M3	315	300	300	300	325
M4	285	285	300	300	350
M5	300	285	300	285	350
M6	300	310	310	300	355
M7	315	315	315	300	355
M8	300	315	300	315	360
M9	285	285	285	300	355
M10	315	315	310	370	370
M11	285	285	300	285	350
M12	420	335	450	455	450
M13	300	300	300	300	345
M14	300	315	300	300	350
M15	300	315	300	300	355
M16	315	305	300	300	345

M17	310	305	300	300	345

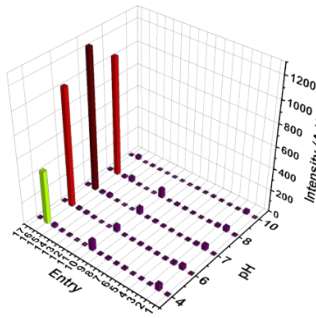
Table S14. The wavelength for maximum absorbance (λ_{abs}) of bDABs (**N1**-**N17**).

	λ_{abs} (nm)				
	pH 4.0	**pH 6.0**	**pH 7.0**	**pH 8.0**	**pH 10.0**
N1	285	300	300	300	340
N2	305	300	300	300	310
N3	325	300	300	300	335
N4	285	300	300	300	350
N5	305	300	300	300	310
N6	285	300	300	300	310
N7	285	300	300	300	350
N8	285	300	300	300	310
N9	285	300	300	300	310
N10	310	310	310	310	365
N11	285	300	300	300	345
N12	365	410	415	460	460
N13	305	300	300	300	310
N14	285	300	300	300	310
N15	310	300	300	300	350
N16	310	310	310	315	310
N17	310	300	300	300	310

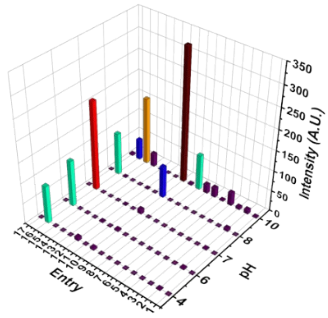
3. Results of primary screening for fluorescence response of a bDAB library (A1-N17) under pH conditions



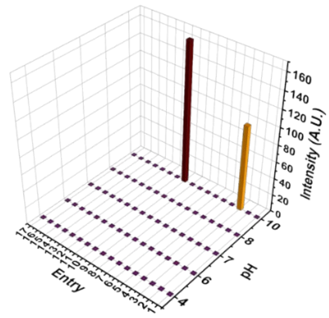
A1-17



λ_{Ex}: 300 nm

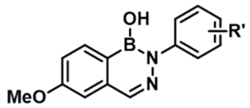


λ_{Ex}: 350 nm

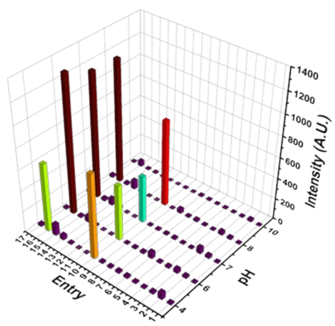


λ_{Ex}: 400 nm

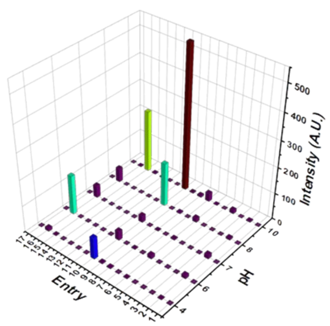
Figure S13. Change of fluorescence intensity of bDABs (**A1**-**17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.



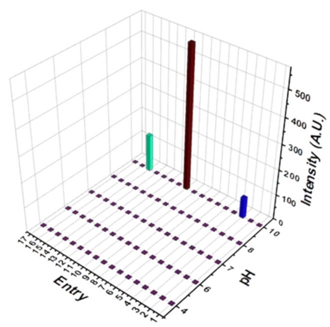
B1-17



λ_{Ex}: 300 nm

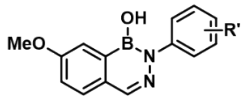


λ_{Ex}: 350 nm

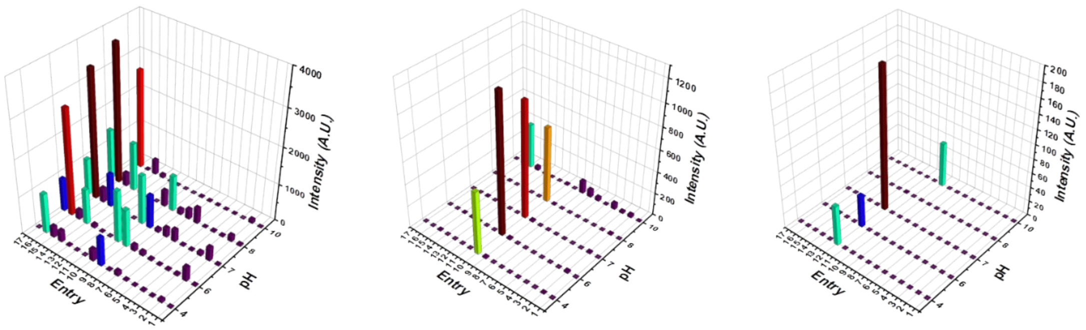


λ_{Ex}: 400 nm

Figure S14. Change of fluorescence intensity of bDABs (**B1**-**17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) at based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

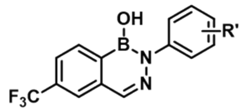


C1-17

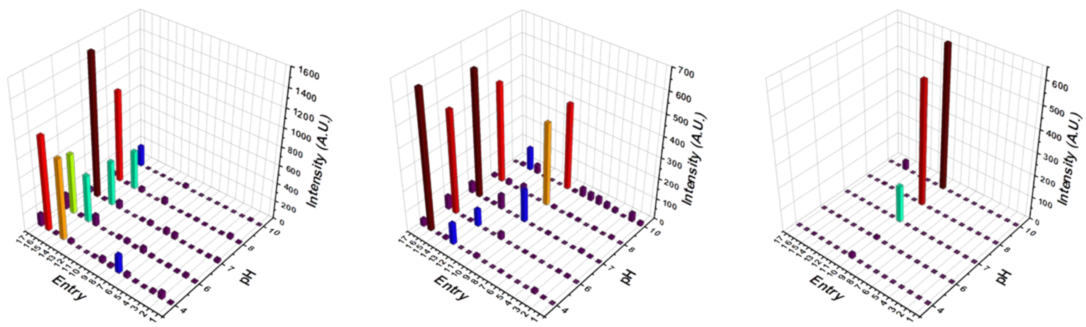


λ_{Ex}: 300 nm λ_{Ex}: 350 nm λ_{Ex}: 400 nm

Figure S15. Change of fluorescence intensity of bDABs (**C1-17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

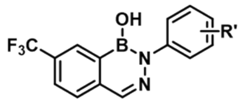


D1-17

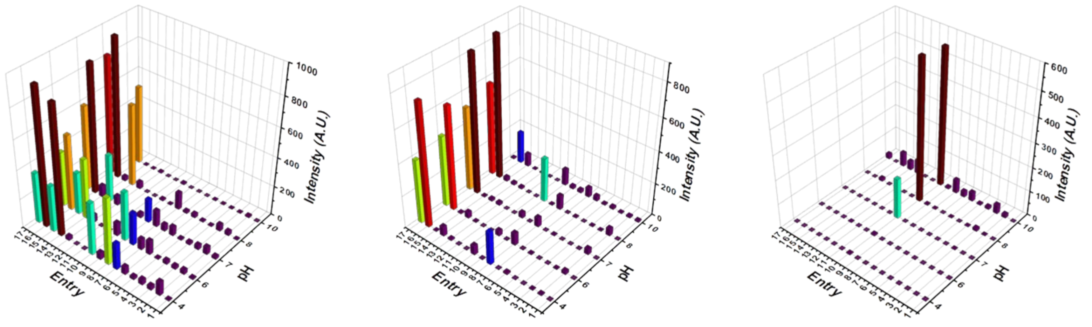


λ_{Ex}: 300 nm λ_{Ex}: 350 nm λ_{Ex}: 400 nm

Figure S16. Change of fluorescence intensity of bDABs (**D1-17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

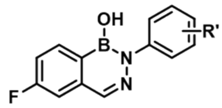


E1-17

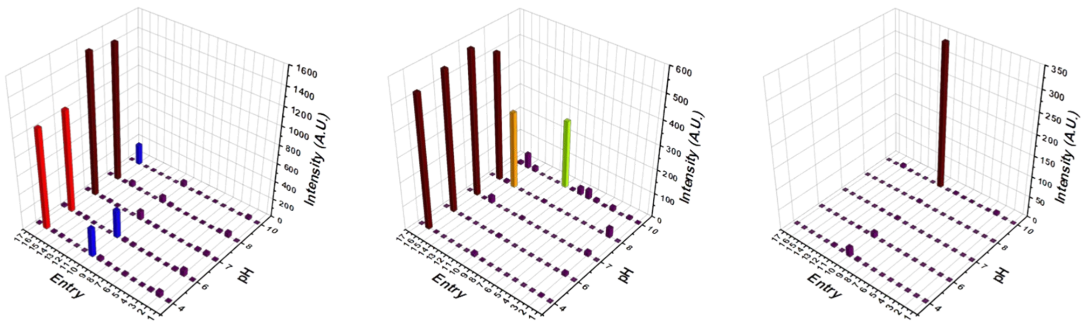


λ_{Ex}: 300 nm λ_{Ex}: 350 nm λ_{Ex}: 400 nm

Figure S17. Change of fluorescence intensity of bDABs (**E1**-**17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

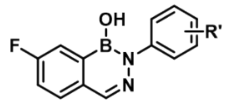


F1-17

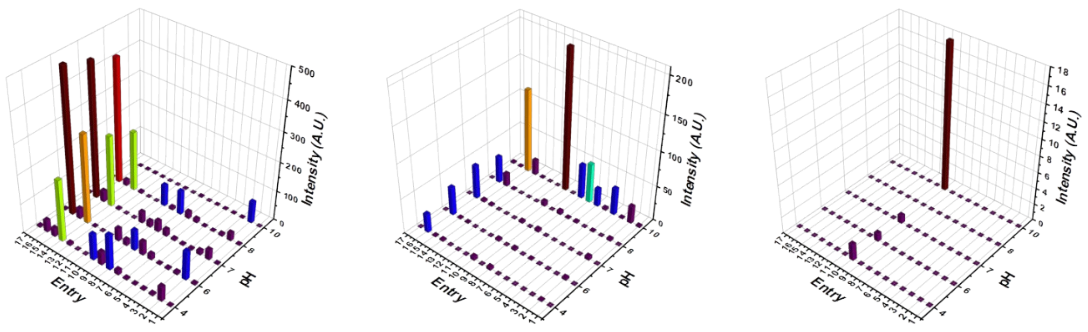


λ_{Ex}: 300 nm λ_{Ex}: 350 nm λ_{Ex}: 400 nm

Figure S18. Change of fluorescence intensity of bDABs (**F1**-**17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

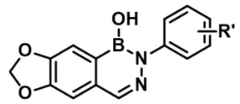


G1-17

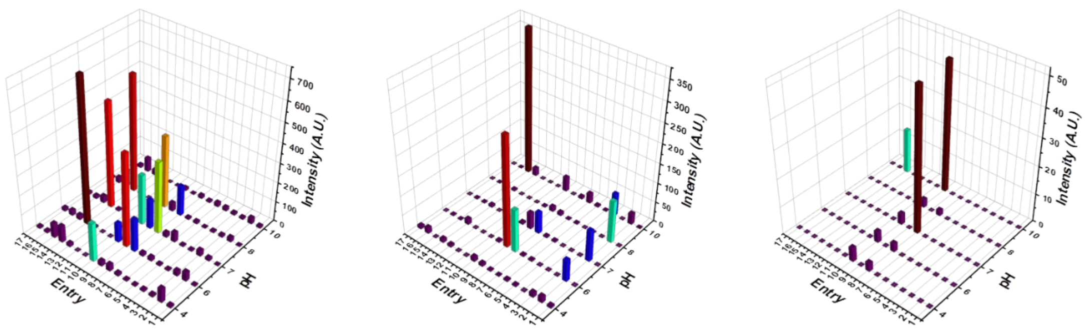


λ_{Ex}: 300 nm λ_{Ex}: 350 nm λ_{Ex}: 400 nm

Figure S19. Change of fluorescence intensity of bDABs (**G1-17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

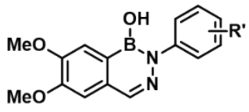


H1-17

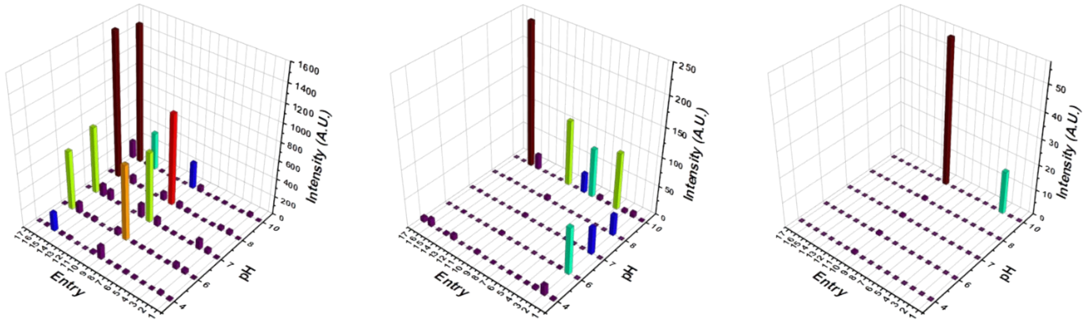


λ_{Ex}: 300 nm λ_{Ex}: 350 nm λ_{Ex}: 400 nm

Figure S20. Change of fluorescence intensity of bDABs (**H1-17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

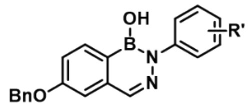


I1-17

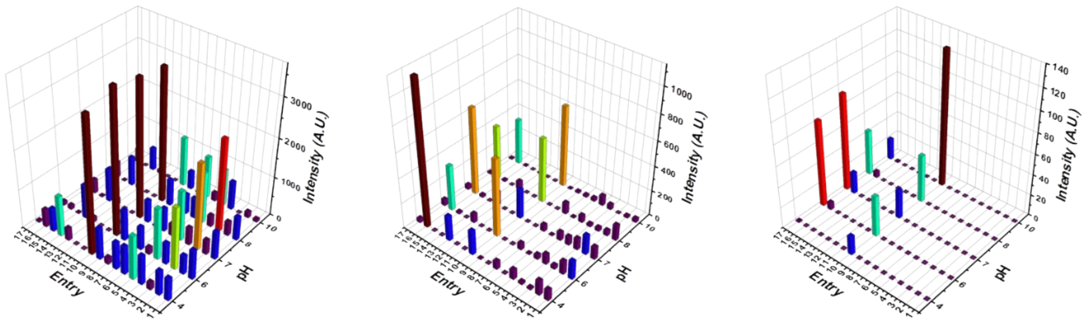


λ_{Ex}: 300 nm | λ_{Ex}: 350 nm | λ_{Ex}: 400 nm

Figure S21. Change of fluorescence intensity of bDABs (**I1**-**17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

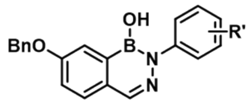


J1-17

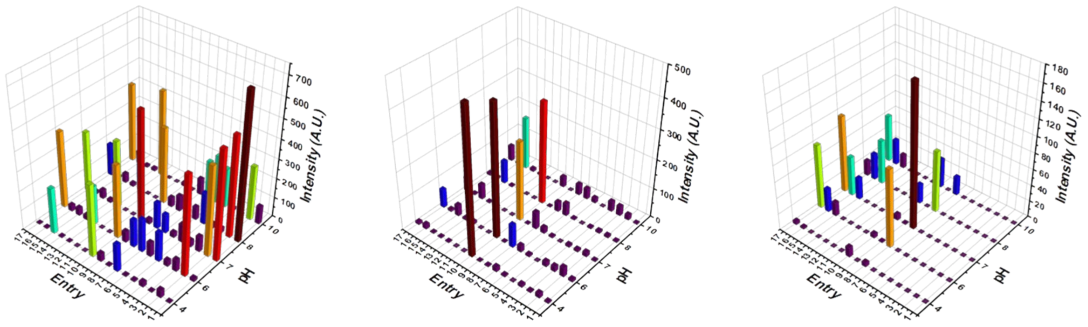


λ_{Ex}: 300 nm | λ_{Ex}: 350 nm | λ_{Ex}: 400 nm

Figure S22. Change of fluorescence intensity of bDABs (**J1**-**17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

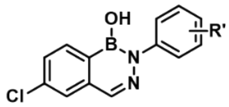


K1-17

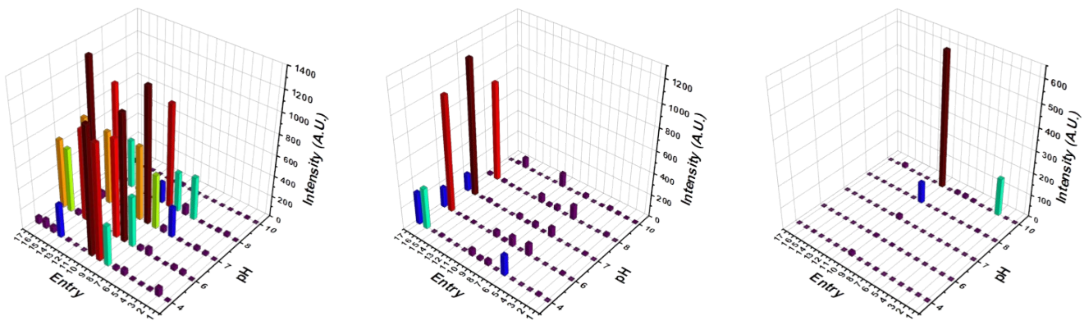


λ$_{Ex}$: 300 nm λ$_{Ex}$: 350 nm λ$_{Ex}$: 400 nm

Figure S23. Change of fluorescence intensity of bDABs (**K1**-**17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

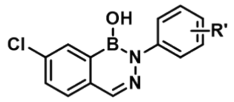


L1-17

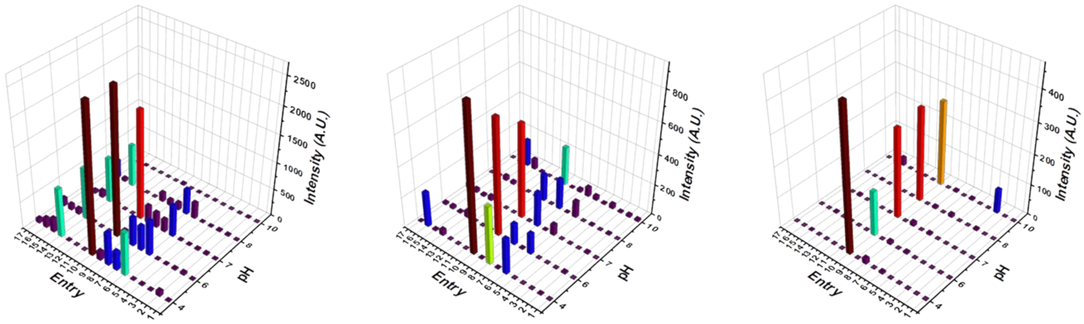


λ$_{Ex}$: 300 nm λ$_{Ex}$: 350 nm λ$_{Ex}$: 400 nm

Figure S24. Change of fluorescence intensity of bDABs (**L1**-**17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

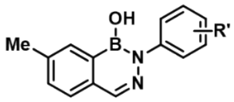


M1-17

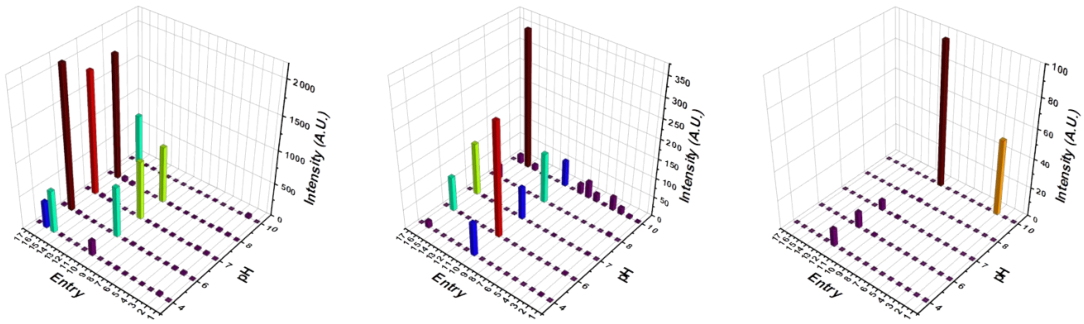


λ_{Ex}: 300 nm λ_{Ex}: 350 nm λ_{Ex}: 400 nm

Figure S25. Change of fluorescence intensity of bDABs (**M1-17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.



N1-17



λ_{Ex}: 300 nm λ_{Ex}: 350 nm λ_{Ex}: 400 nm

Figure S26. Change of fluorescence intensity of bDABs (**N1-17**) by a change of pH under 3 different λ_{ex} (300/350/400 nm) based on λ_{em} (emission wavelength of maximum intensity) at pH 4, [bDAB] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

Table S15. Fluorescence intensity at respective wavelength (λ_{em}) of **E14** by a change of pH under three different λ_{ex}, [**E14**] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

λ_{ex}	λ_{em}	pH 4.0	pH 6.0	pH 7.0	pH 8.0	pH 10.0
300 nm	410 nm	879	411	327	565	2
350 nm	405 nm	59	38	15	14	2
400 nm	485 nm	0	0	0	0	37

Table S16. Fluorescence intensity at respective wavelength (λ_{em}) of **I16** by a change of pH under three different λ_{ex}, [**I16**] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

λ_{ex}	λ_{em}	pH 4.0	pH 6.0	pH 7.0	pH 8.0	pH 10.0
300 nm	355 nm	11	651	740	1587	1515
350 nm	450 nm	13	0	1	0	0
400 nm	500 nm	0	0	0	0	0

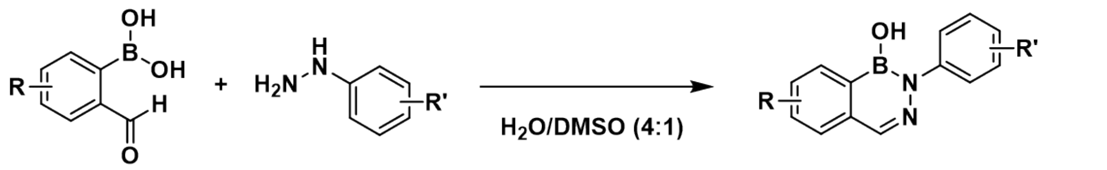
Table S17. Fluorescence intensity at respective wavelength (λ_{em}) of **J7** by a change of pH under three different λ_{ex}, [**J7**] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

λ_{ex}	λ_{em}	pH 4.0	pH 6.0	pH 7.0	pH 8.0	pH 10.0
300 nm	380 nm	697	594	602	511	1075
350 nm	405 nm	63	52	53	92	18
400 nm	500 nm	0	0	0	0	0

Table S18. Fluorescence intensity at respective wavelength (λ_{em}) of **L10** by a change of pH under three different λ_{ex}, [**L10**] = 100 μM in 20 mM buffers pH 4.0 citrate; pH 6.0 phosphate; pH 7.0 phosphate; pH 8.0 phosphate; pH 10.0 carbonate with 10% DMSO.

λ_{ex}	λ_{em}	pH 4.0	pH 6.0	pH 7.0	pH 8.0	pH 10.0
300 nm	450 nm	1210	942	718	205	19
350 nm	450 nm	57	55	38	71	124
400 nm	450 nm	17	6	19	96	611

4. Synthesis and characterization of four bDABs (E14, I16, J7, L10)



E14 : **R** = 5-CF$_3$, **R'** = 4-OCF$_3$
I16 : **R** = 4,5-diOMe, **R'** = 4-*i*-Pr
J7 : **R** = 4-OBn, **R'** = 3-Br
L10 : **R** = 4-Cl, **R'** = 4-CN

Scheme S1. Synthesis of four bDABs (**E14**, **I16**, **J7**, **L10**).

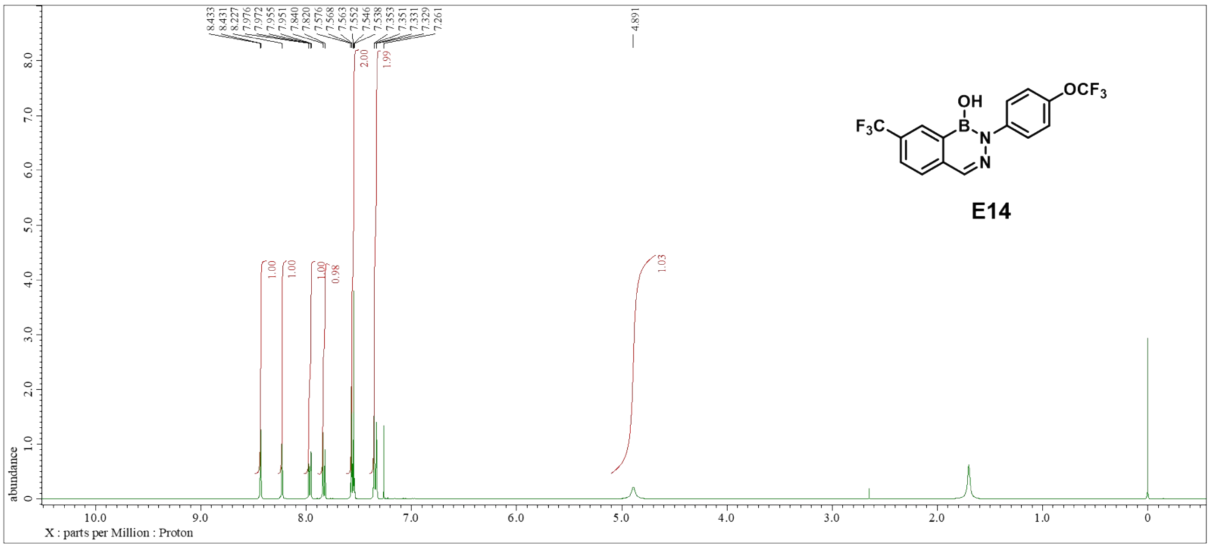


Figure S27. ^{1}H NMR spectrum (400 MHz, CHLOROFORM-D) of **E14**.

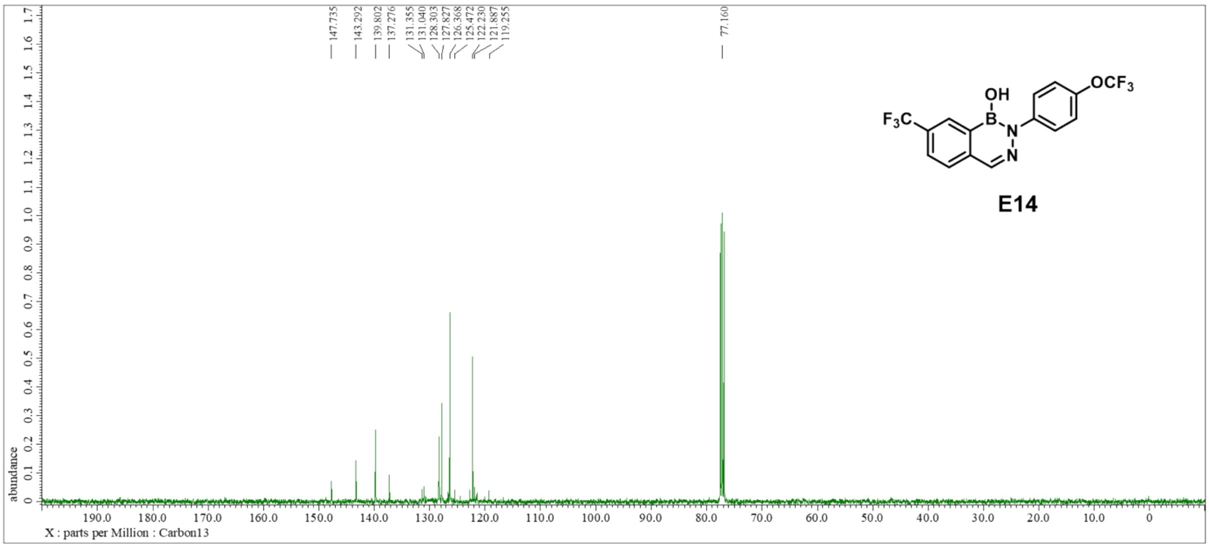


Figure S28. ^{13}C NMR spectrum (101 MHz, CHLOROFORM-D) of **E14**.

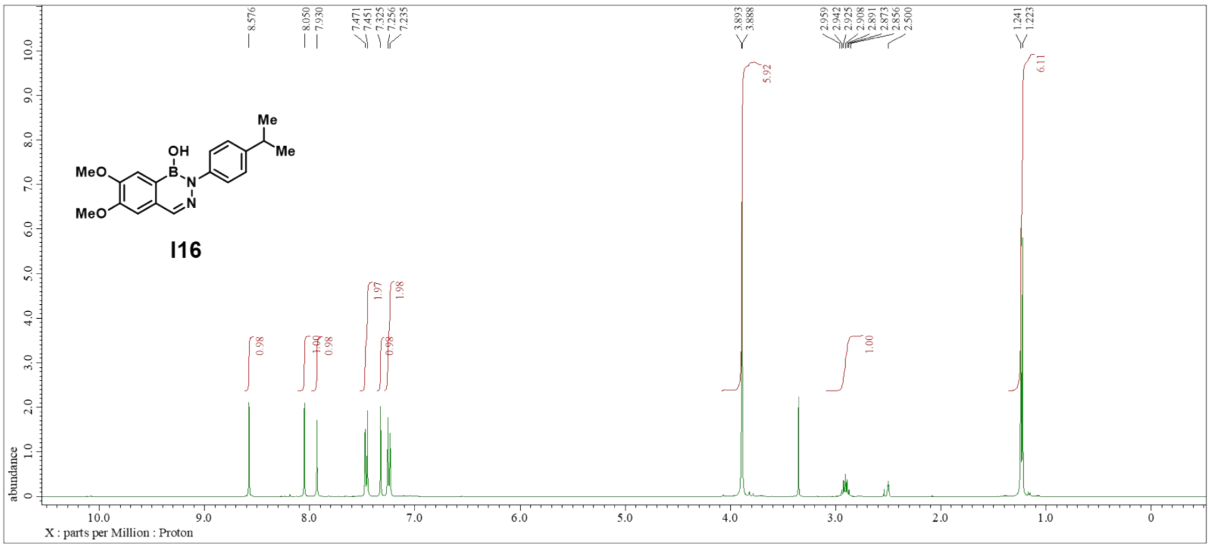


Figure S29. ^{1}H NMR spectrum (400 MHz, DMSO-D6) of **I16**.

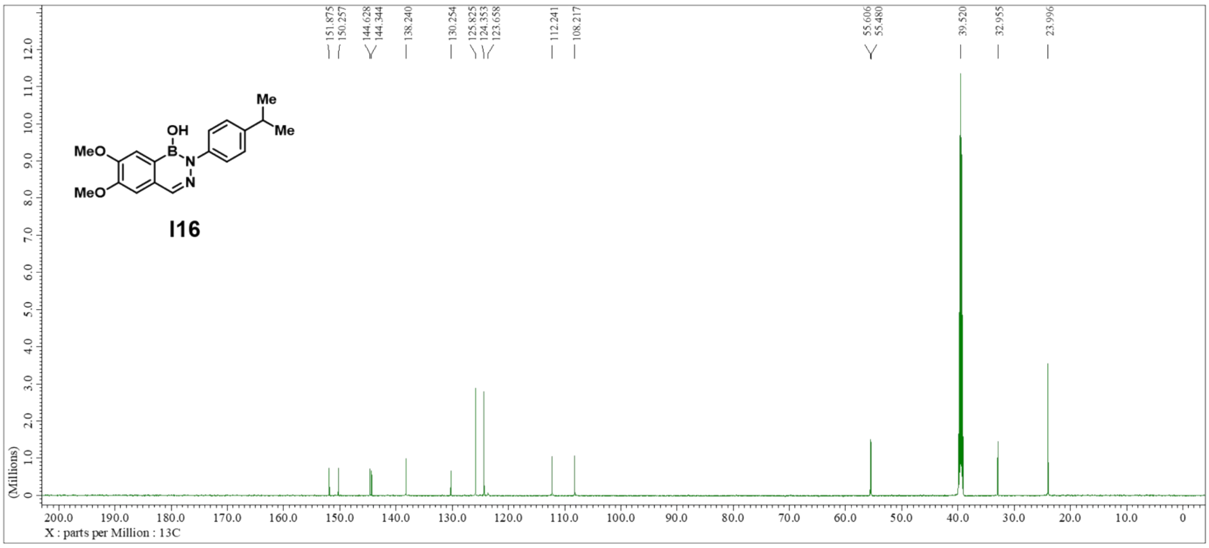


Figure S30. ^{13}C NMR spectrum (151 MHz, DMSO-D6) of **I16**.

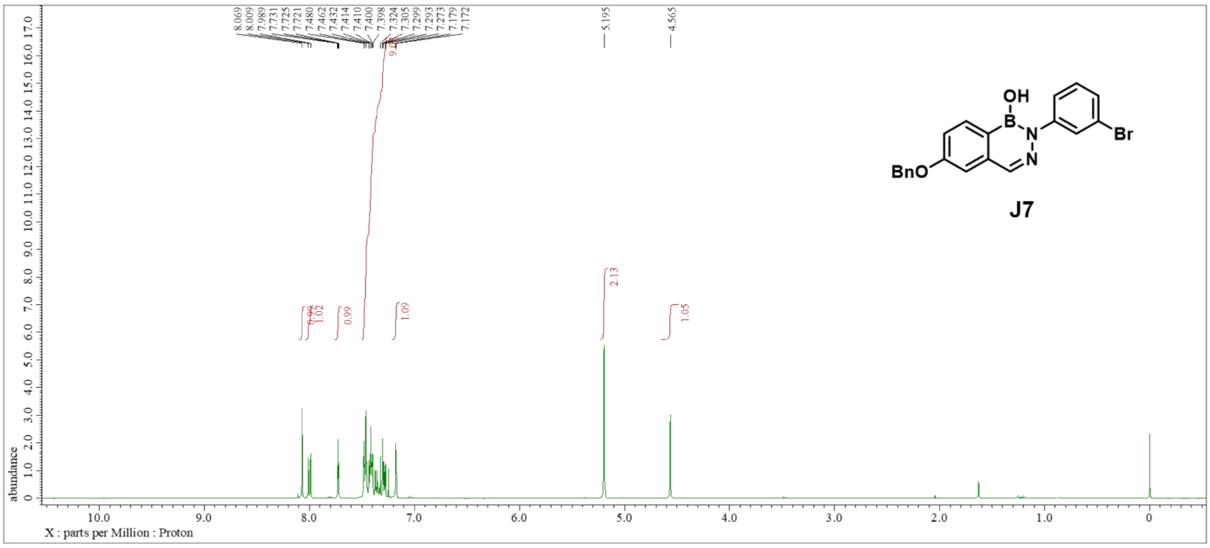


Figure S31. ^{1}H NMR spectrum (400 MHz, CHLOROFORM-D) of **J7**.

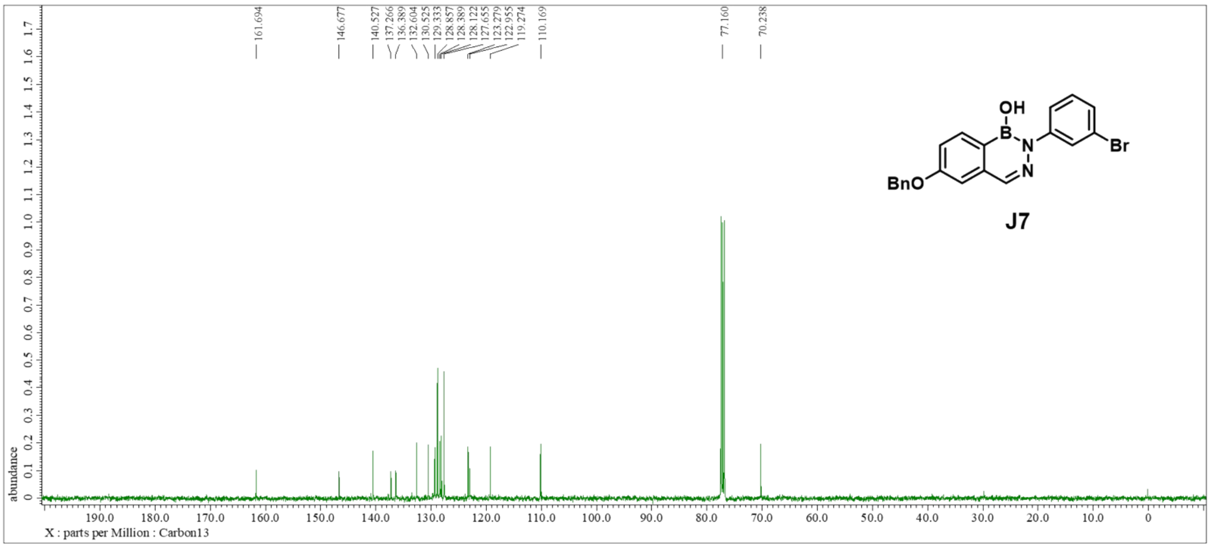


Figure S32. ^{13}C NMR spectrum (101 MHz, CHLOROFORM-D) of **J7**.

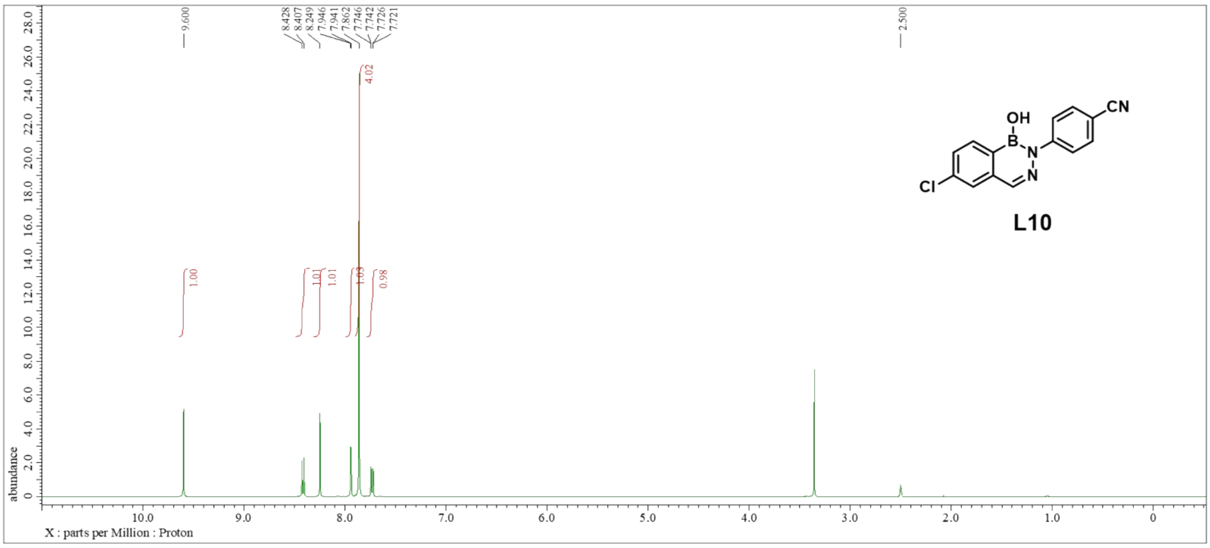


Figure S33. ^{1}H NMR spectrum (400 MHz, DMSO-D6) of **L10**.

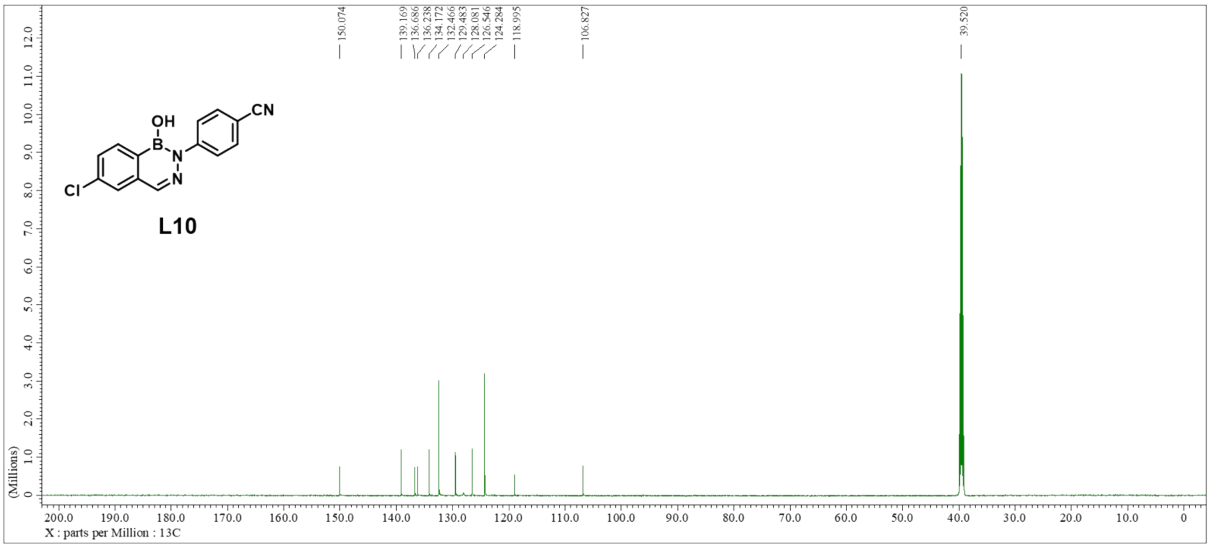


Figure S34. ^{13}C NMR spectrum (151 MHz, DMSO-D6) of **L10**.

5. Results of secondary screening for fluorescence response of bDABs (I16, J7, L10) under varied pH conditions

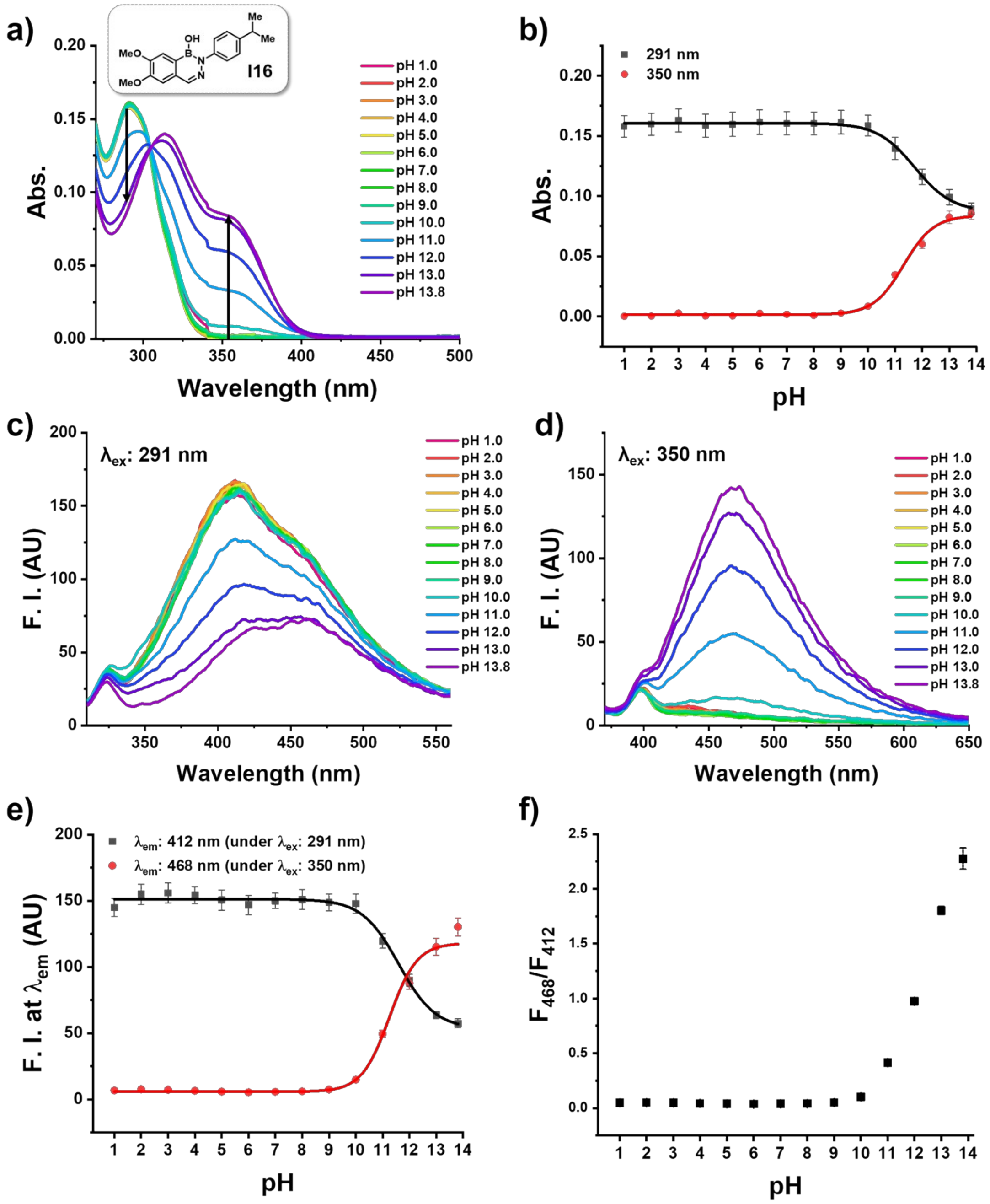


Figure S35. The change of optical properties of **I16** (10 μM) under the pH variations (pH 1.0-13.8), a) and b) UV/vis spectral change, c, d), and e) fluorescence spectral change, f) plot of F_{468}/F_{412} versus pH value, where F_{468} and F_{412} are emission values at wavelengths of 468 and 412 nm, respectively.

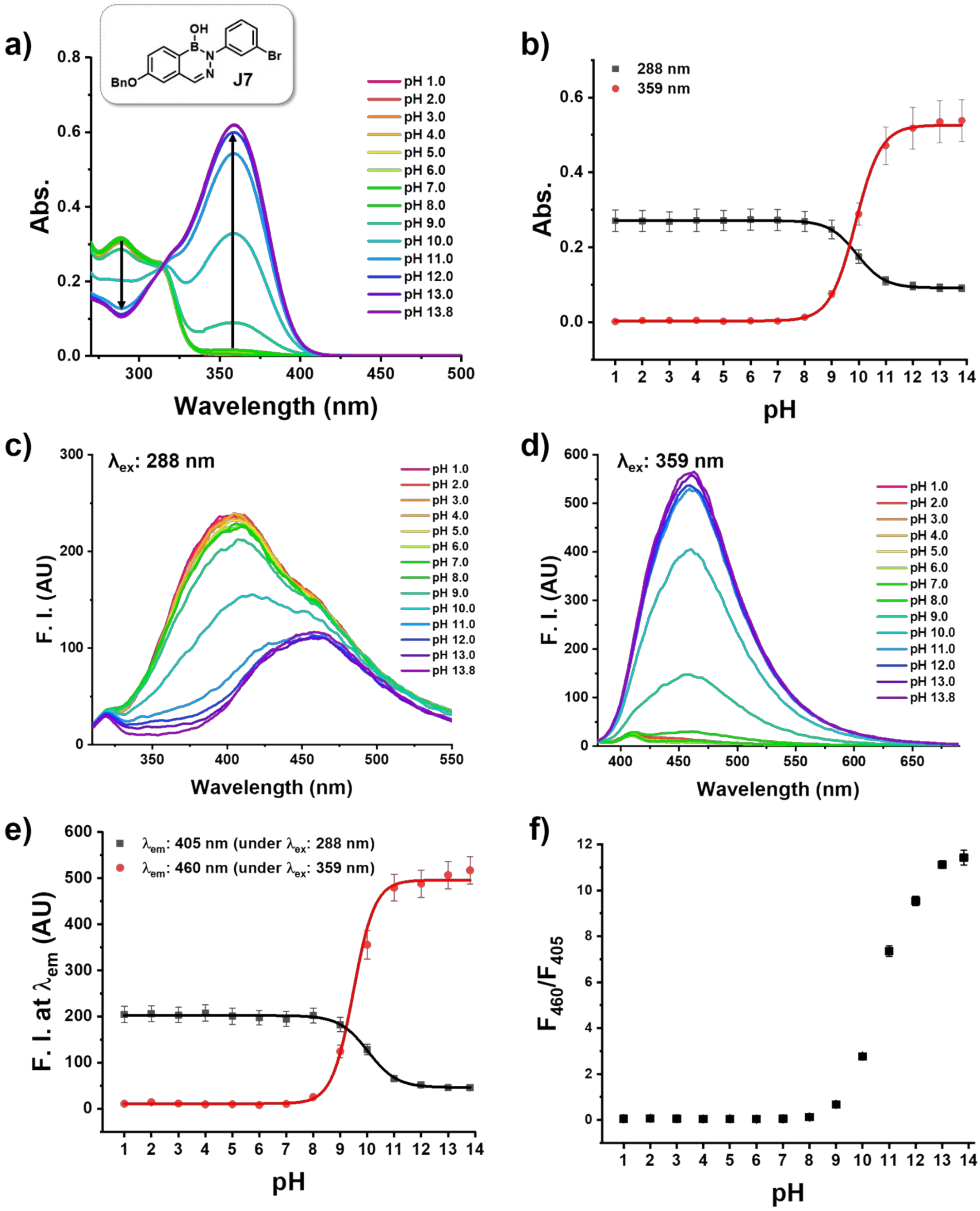


Figure S36. The change of optical properties of **J7** (25 μM) under the pH variations (pH 1.0-13.8), a) and b) UV/vis spectral change, c, d), and e) fluorescence spectral change, f) plot of F_{460}/F_{405} versus pH value, where F_{460} and F_{405} are emission values at wavelengths of 460 and 405 nm, respectively.

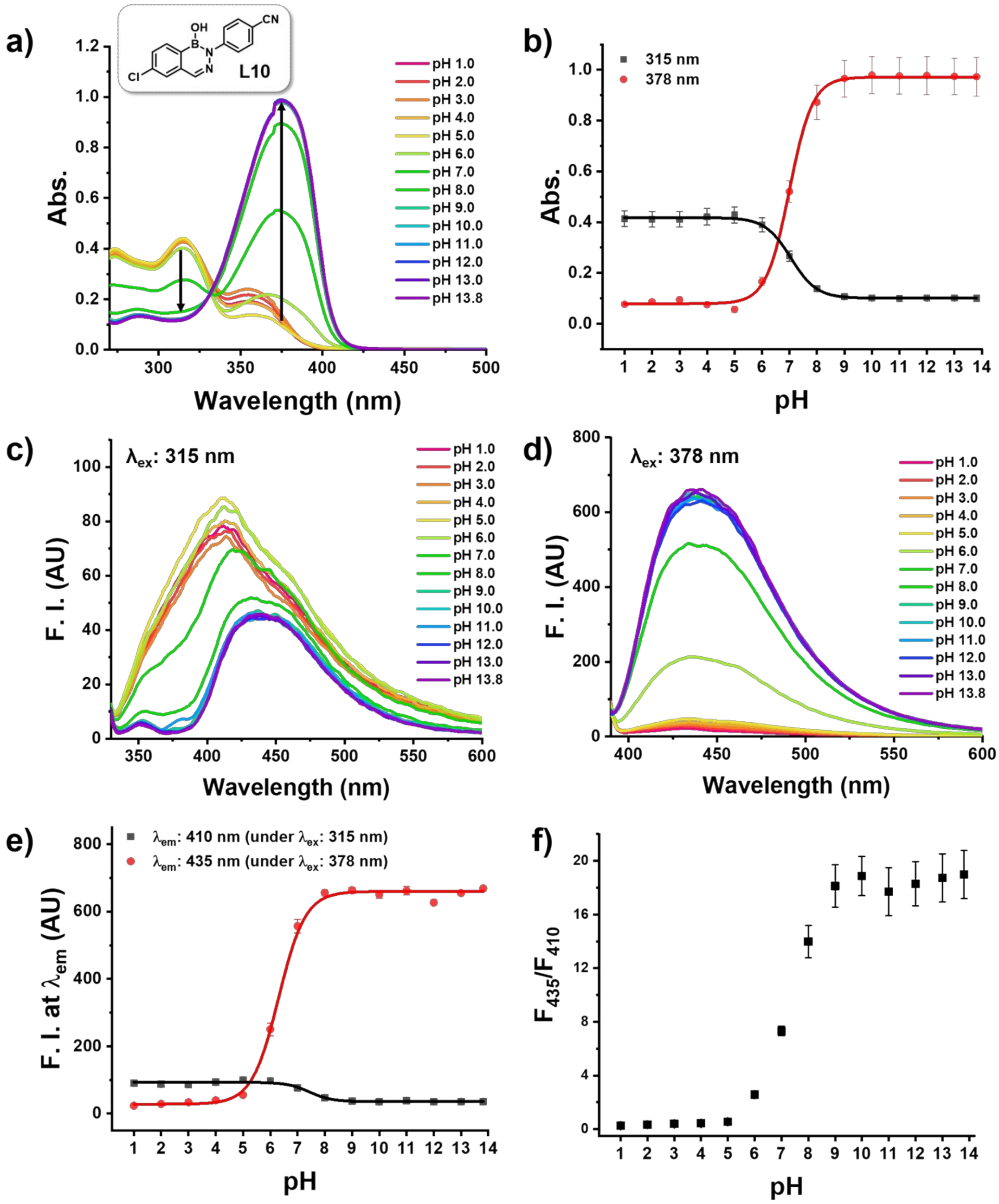


Figure S37. The change of optical properties of **L10** (25 μM) under the pH variations (pH 1.0-13.8), a) and b) UV/vis spectral change, c, d), and e) fluorescence spectral change, f) plot of F_{435}/F_{410} versus pH value, where F_{435} and F_{410} are emission values at wavelengths of 435 and 410 nm, respectively.

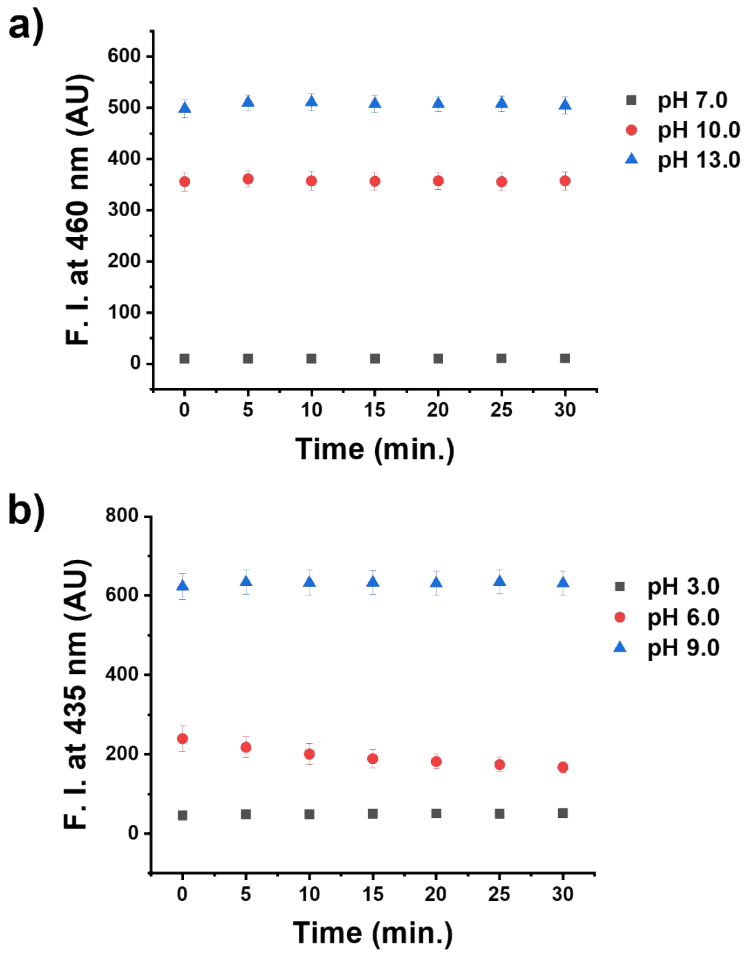


Figure S38. Plot of the fluorescence intensities of a) **J7** (25 μM) and b) **L10** (25 μM) under three different pH conditions over a period of 30 min, λ_{ex} = 359, 378 nm, respectively.

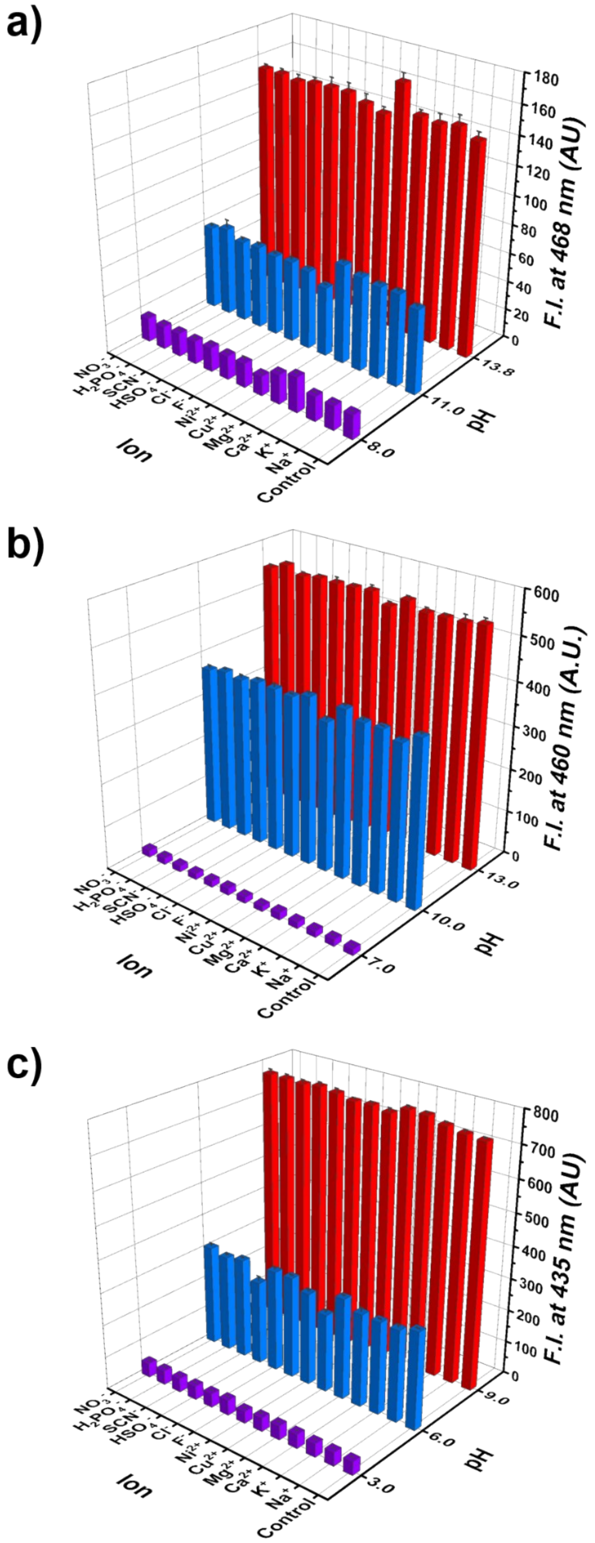


Figure S39. Fluorescence intensity of a) **I16** (10 μM), b) **J7** (25 μM), and c) **L10** (25 μM) at three different pH condition in the absence (control) and presence of various ion species (Na^+: 10 mM; K^+: 10 mM; Ca^{2+}: 1 mM; Mg^{2+}: 1 mM; Cu^{2+}: 1 mM; Ni^{2+}: 1 mM; F^-: 1 mM; Cl^-: 1 mM; HSO_4^-: 1 mM; SCN^-: 1 mM; $H_2PO_4^-$: 1 mM; NO_3^-: 1 mM), λ_{ex} =350, 359, 378 nm, respectively.

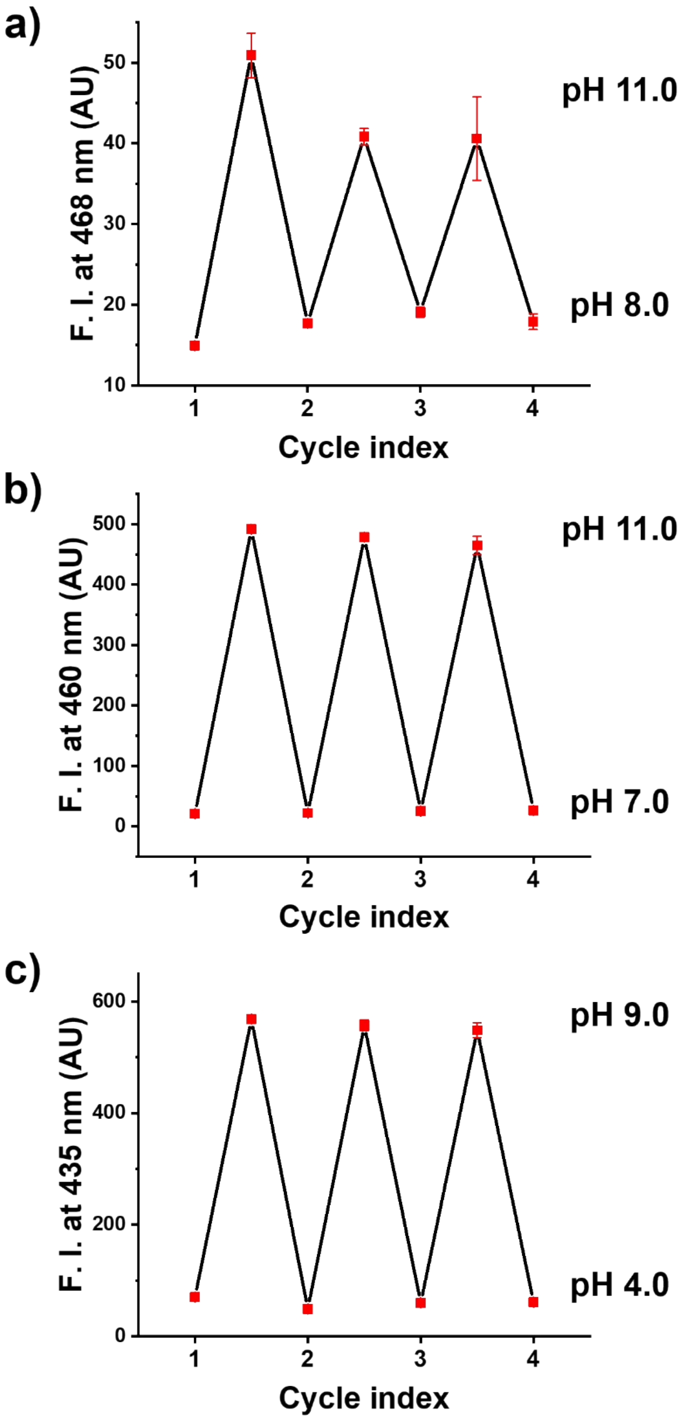


Figure S40. Reversibility of fluorescence response of a) **I16** (10 μM), b) **J7** (25 μM), and c) **L10** (25 μM) between low pH and high pH, λ_{ex} =350, 359, 378 nm, respectively.