Supporting Information

Direct discrimination of cell surface glycosylation signatures using a single pH-responsive boronic acid-functionalized polymer

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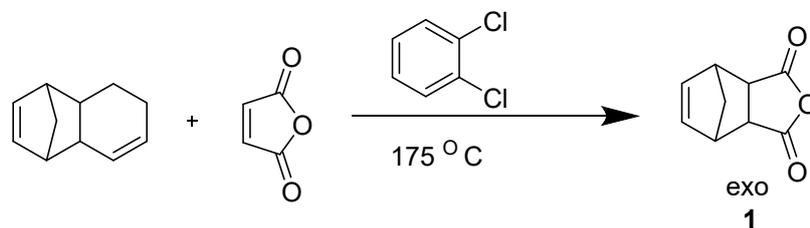
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[+]M. Jiang and A. N. Chattopadhyay contributed equally to the work.

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1. Synthesis of PONI-boronic acid (BA)-pyrene (PONI-BA-Pyrene)

The **PONI-BA-Pyrene** polymer was synthesized according to the following protocols.

Synthesis of **1**

24.5 g of dicyclopentadiene was melted in hot water (185 mmol, 1.0 eq) at 50°C for 10 minutes. 30 g of maleic anhydride (370 mmol, 2.0 eq) was brought to reflux in 60 mL of o-dichlorobenzene in a 250 mL round bottom flask. The liquid dicyclopentadiene was then transferred to the reaction flask dropwise over a time of 15 minutes. The reaction was left to run at reflux for another 1.5 hours. After that, the reaction was taken off the heat and allowed to cool down to room temperature. After 2 hours, the flask was transferred to the refrigerator to be kept overnight for cooling down. 12 hours later, the resulting crystalline solid was filtered off in vacuo. Multiple recrystallizations in boiling monochlorobenzene resulted in the isolation of the desired compound **1** with a high exo purity in a yield of 45%. ^{1}H NMR (400 MHz, CDCl$_3$) 6.34 (s, 2H), 3.45 (s, 2H), 3.01 (s, 2H), 1.79 (d, J=11Hz, 2H), 1.57 (d, J=11Hz, 2H), p.p.m.
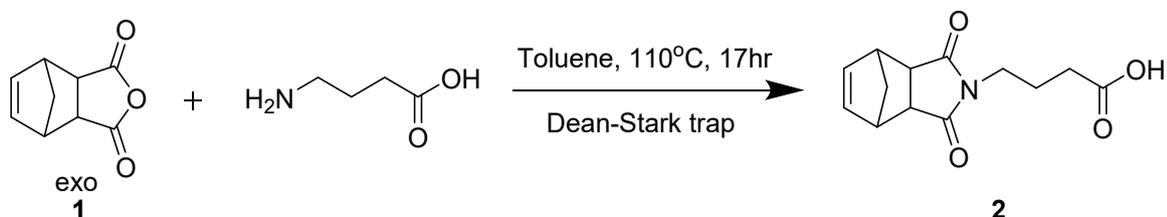
Synthesis of **2**

To a 250 mL round bottom flask equipped with a stir bar was added 50 mL of toluene. Next, **1** (1 g, 6.09 mmol, 1.0 eq) was added along with 4-aminobutyric acid (0.69 g, 6.70 mmol, 1.1 eq). The reaction mixture was connected to a Dean-Stark trap and heated to 110 °C and it was left to run overnight. Afterwards, the reaction mixture was cooled down to room temperature, washed with 1M HCl (3x, 30 mL), water (3x, 30 mL) and brine (1x, 30 mL). The organic layer was dried with sodium sulfate, filtered and rotavaped. Column chromatography was performed to yield **2** as a white solid (76% yield). ^{1}H NMR (400 MHz, CDCl$_3$) 6.32 (s, 2H), 3.55 (t, 2H), 3.28 (s, 2H), 2.70 (s, 2H), 2.39 (t, 2H), 1.92 (q, 2H), 1.53 (m, 1H), 1.21 (m, 1H).
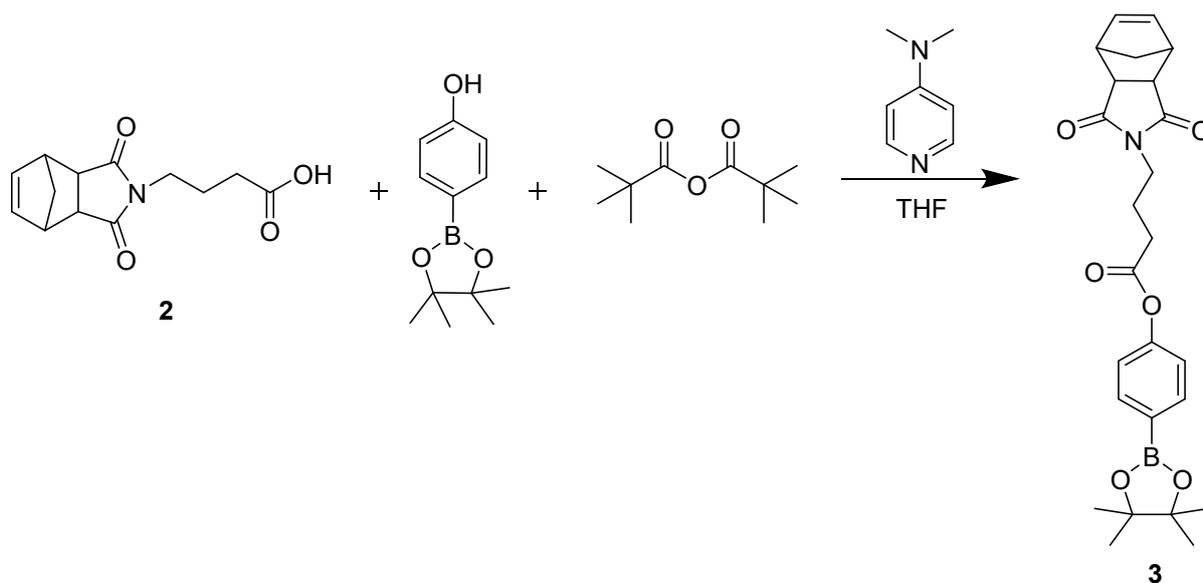
Synthesis of 3

2 (1.1 g, 4.4 mmol, 1.1 eq), 4-hydroxyphenylboronic acid pinacol ester (0.9 g, 4.0 mmol, 1.0 eq) and 4-dimethylaminopyridine was mixed with dry THF and refluxed in a 250 ml round bottom flask. The mixture was stirred until everything got dissolved. After the solution was clear, pivalic anhydride (0.8 g, 4.4 mmol, 1.1 eq) was added to the reaction mixture. The reaction was kept stirring for 24 hours at reflux condition. After 24 hours, 5 ml of water was added to the reaction and stirred for 2 hours. Dichloromethane was added to the reaction mixture, washed with saturated sodium bicarbonate (3x) and brine (1x) and dried over $MgSO_4$. The mixture was filtered and concentrated on a rotary evaporator. Column chromatography was done in silica with 33% ethyl acetate in hexanes which resulted in a white solid (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$) 7.82 (d, 2H), 7.10 (d, 2H), 6.27 (s, 2H), 3.61 (t, 2H), 3.28 (s, 2H), 2.69 (s, 2H), 2.58 (t, 2H), 2.00 (m, 2H), 1.55 (m, 2H), 1.33 (s, 12H).
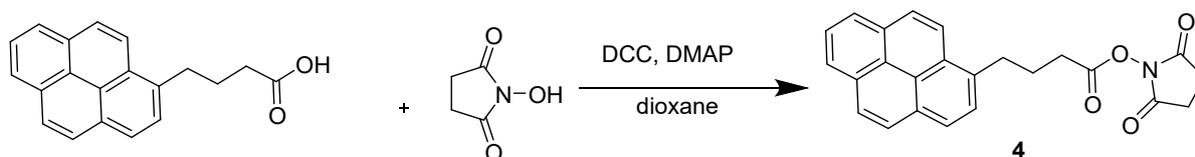
Synthesis of 4

Pyrene butyric acid (2.0 g, 4.4 mmol, 1.1 eq) and N-hydroxysuccinimide (0.9 g, 4.0 mmol, 1.0 eq) were mixed and dissolved in dioxane in an ice bath. Dicyclohexylcarbodiimide was added to the mixture at 0 °C and the reaction mixture was stirred for 15 mins. 4-dimethylaminopyridine was next added to the mixture at 0 °C and stirred for 1 hr in the ice bath. After 1 hr, the ice bath was removed, and the reaction was left to run overnight. After 18 hrs, the reaction was stopped, and the mixture was concentrated on a rotary evaporator. Column chromatography in silica with 50% ethyl acetate in hexanes yielded **4** as a yellowish white solid (37% yield). ^{1}H NMR (400 MHz, $CDCl_3$) 8.30 (d, 1H), 8.15 (m, 4H), 8.00 (m, 3H), 7.88 (d, 1H), 3.45 (t, 2H), 2.90 (s, 4H), 2.84 (t, 2H), 2.30 (p, 2H).
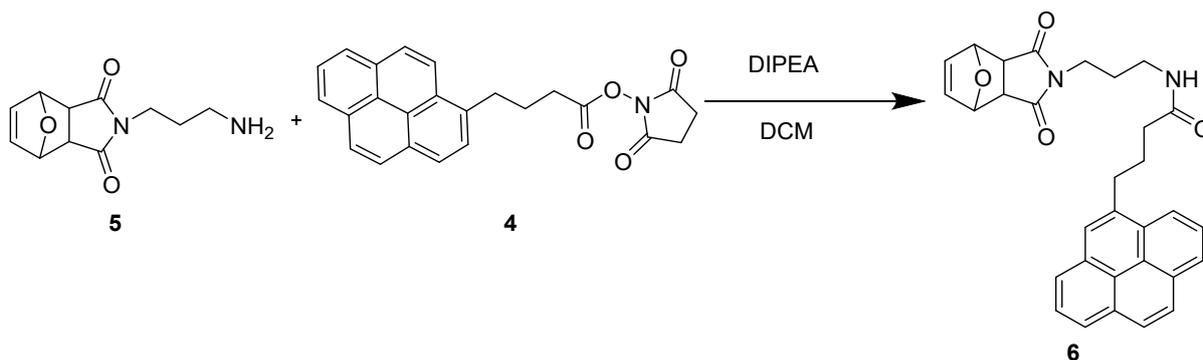
Synthesis of 6

Monomer **5** was synthesized following previous reports.[1] **5** (0.60 g, 1.78 mmol, 1.0 eq) was added to a 250 ml round bottom flask equipped with a stir bar under N_2 atmosphere at room temperature. Diisopropylethylamine (0.69 g, 5.35 mmol, 3.0 eq) and dichloromethane was added to the flask under N_2 purging and the mixture was stirred. **4** (0.69 g, 1.78 mmol, 1.0 eq) was slowly added to the reaction and the mixture was stirred for 4 hr at room temperature. Column chromatography was done in silica in pure ethyl acetate to get the product as a slight yellow solid (63% yield). ^{1}H NMR (400 MHz, $CDCl_3$) 8.34 (d, 1H), 8.18 (m, 4H), 8.00 (m, 3H), 7.88 (d, 1H), 6.48 (s, 2H), 6.17 (s, 1H), 5.21 (s, 2H), 3.54 (t, 2H), 3.42 (t, 2H), 3.18 (m, 2H), 2.39 (t, 2H), 2.25 (m, 2H), 1.76 (m, 2H), 1.60 (s, 1H).
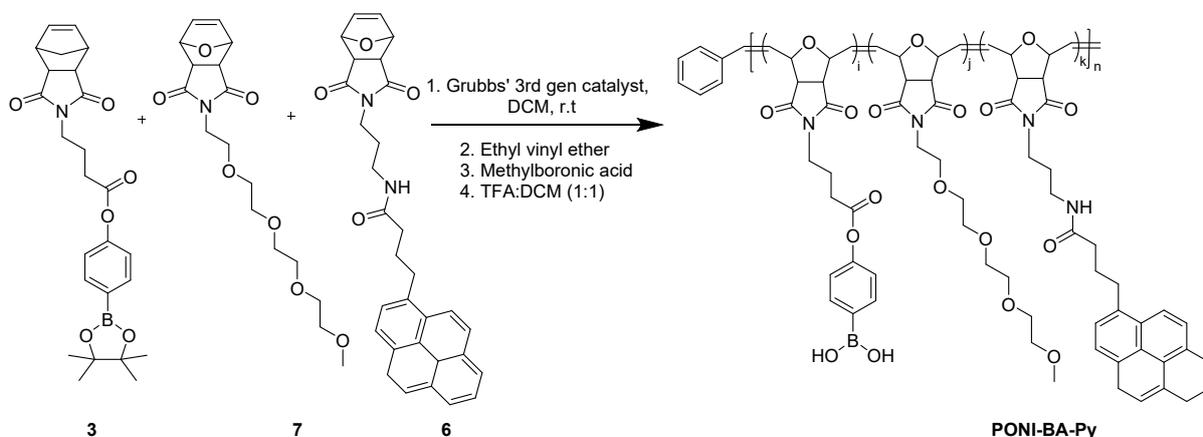
Polymer synthesis scheme:

Monomer **7** was also synthesized following previous reports.[1] To a 15 mL pear-shaped air-free flask equipped with a stir bar was added **3** (50 mg, 0.10 mmol, 2.0 eq), **7** (126 mg, 0.33 mmol, 7.0 eq), **6** (25 mg, 0.05 mmol, 1.0 eq) and 5 mL of DCM. In a separate 10 ml pear-shaped air-free flask was added Grubbs' 3rd generation catalyst (10.0 mg, 0.012 mmol) and 1 mL DCM. Both flasks were sealed with septa and attached to a Schlenk nitrogen/vacuum line. Both flasks were freeze-pump-thawed three times. After thawing, Grubbs' 3rd generation catalyst was removed via syringe and quickly added to the flask containing **3, 7 & 6** and allowed to react for 90 mins. After the allotted time, ethyl vinyl ether (300 μL) was added and allowed to stir for 20 mins. Afterwards, the reaction was diluted to two times the volume and precipitated into a heavily stirred solution of a 1:1 mixture of ethyl ether and hexane. The precipitated polymer

was filtered and dissolved into tetrahydrofuran (THF). The polymer was precipitated again into the same mixture solvent and filtered. After filtration, the residue was dissolved in 5 mL of DCM and 5 mL of trifluoroacetic acid was added to the mixture. Then (160 mg, 5.0 eq) of methylboronic acid was added to the mixture and the reaction was allowed to run overnight. Afterwards, the solvent was completely evaporated and washed with hexane 2 times and dissolved into a minimal amount of water. The polymers were added to 10,000 MWCO dialysis membranes and allowed to stir for 3 days in Milli Q water, changing the water periodically. The polymers were filtered through PES syringe filters and freeze-dried to yield **PONI-BA-Py.** 1H NMR (400MHz, CDCl$_3$) 8.37 (m, 2H), 8.23 (m, 6H), 8.11 (s, 4H), 8.02 (s, 3H), 7.93 (m, 2H), 7.81 (d, 6H), 7.7 (s, 1H), 7.05 (s, 6H), 5.93 (s, 12H), 5.70 (s, 19H), 4.84 (s, 12H), 4.37 (s, 12H), 3.45 (d, 280H), 3.20 (s, 38H), 3.07 (s, 11H), 2.54 (m, 6H), 2.22 (s, 3H), 2.00 (s, 4H), 1.83 (s, 5H), 1.63 (s, 3H), 1.28 (s, 7H). The polymer was also characterized by GPC (gel permeation chromatography) in tetrahydrofuran. The MW was ~30,000 and the PDI (polydispersity index) was 1.01.

2. Characterization of the PONI-BA-Pyrene polymer sensor

2.1 Gel permeation chromatography (GPC)
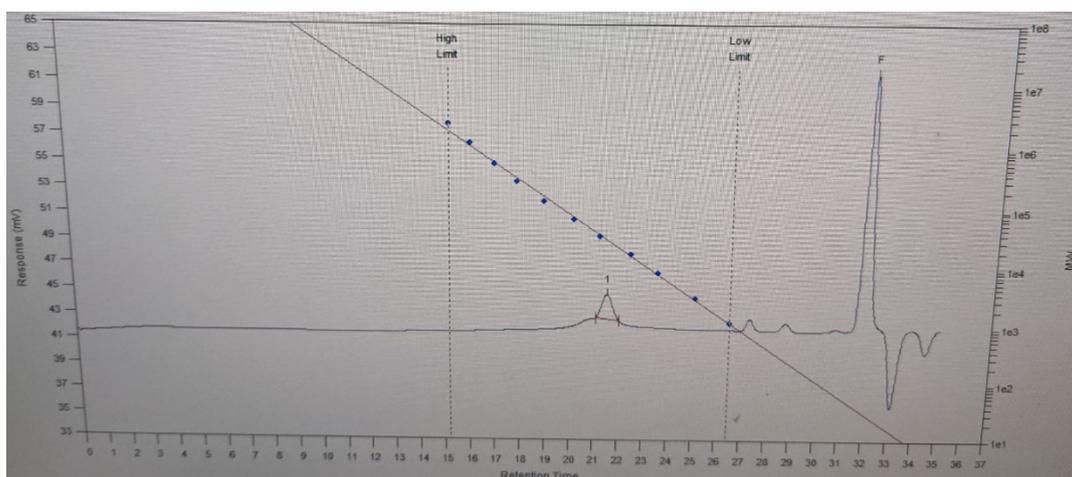
Figure S1. Characterization of Boc-protected polymer using gel permeation chromatography. GPC trace shows that the **PONI-BA-pyrene** has Mw = 30 kDa and Mn = 29.5 kDa and a polydispersity index of 1.01, determined by GPC using polystyrene standards, THF as solvent and toluene as the flow marker.

2.2 Transmission Electron Microscopy (TEM) of PONI-BA-pyrene
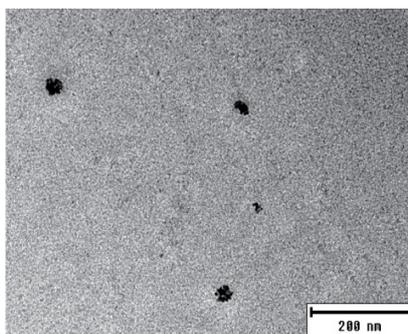
Figure S2. TEM image **of PONI-BA-pyrene** used in the study, which was taken under 30,000x magnification.

2.3 Dynamic light scattering (DLS) of PONI-BA-pyrene
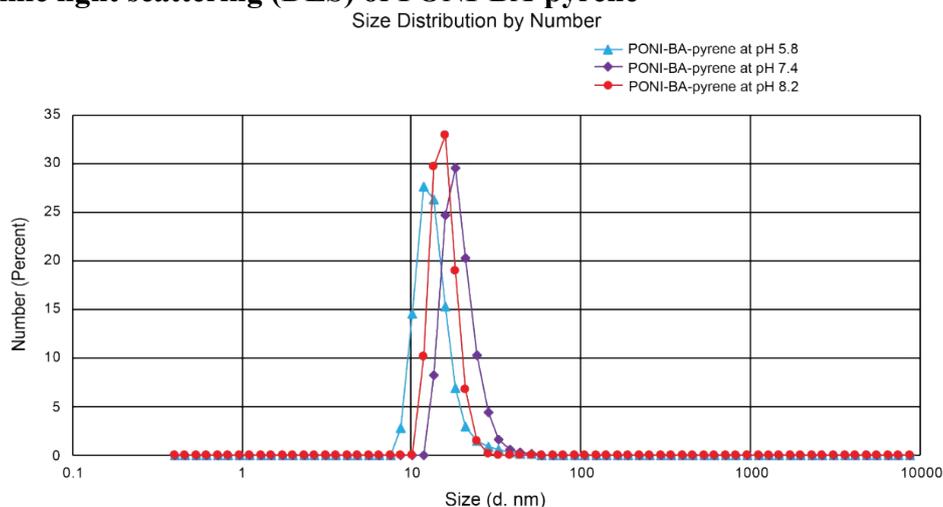
Figure S3. Hydrodynamic sizes of **PONI-BA-pyrene** polymers in 5 mM phosphate buffers with different pH values. The sizes of **PONI-BA-pyrene** under pH 5.8, 7.4, and 8.2 are approximately 14.0 ±5.0, 19.4 ±4.7, and 15.6 ±2.7 nm, respectively, which indicates the size of polymer is stable upon changing pH values.

2.4 Fluorescence response of PONI-BA-pyrene under different pH
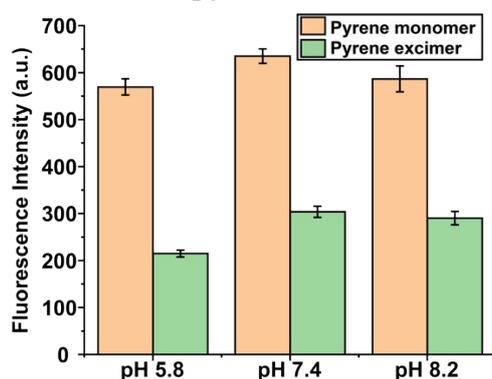
Figure S4. Fluorescence intensities of 40 µg/L **PONI-BA-pyrene** under different pH, with the monomer emission of 398 nm and excimer emission of 473 nm at the excitation of 330 nm. Each value is the average of eight parallel measurements (n=8).

3. Interaction between boronic acid and diol

3.1 Fluorescence response of PONI-BA-pyrene incubating with different concentrations of saccharides
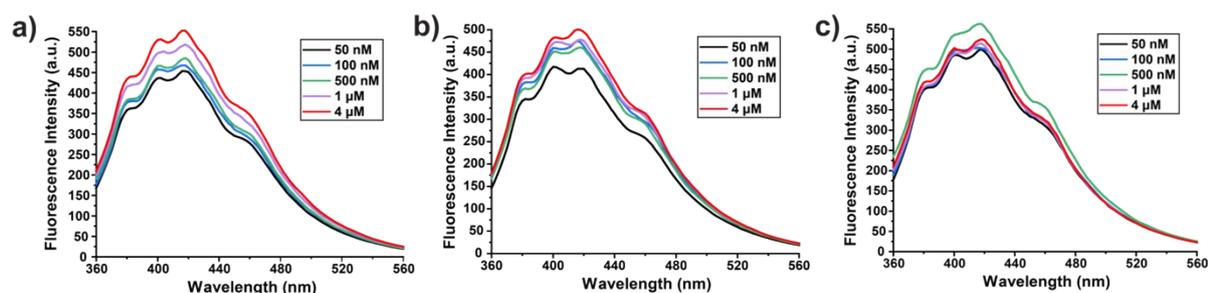
3.2 FT-IR studies with noroborneneimide-based boronic acid monomer

Synthesis of norborneneimide-based boronic acid monomer (**NI-BA**):
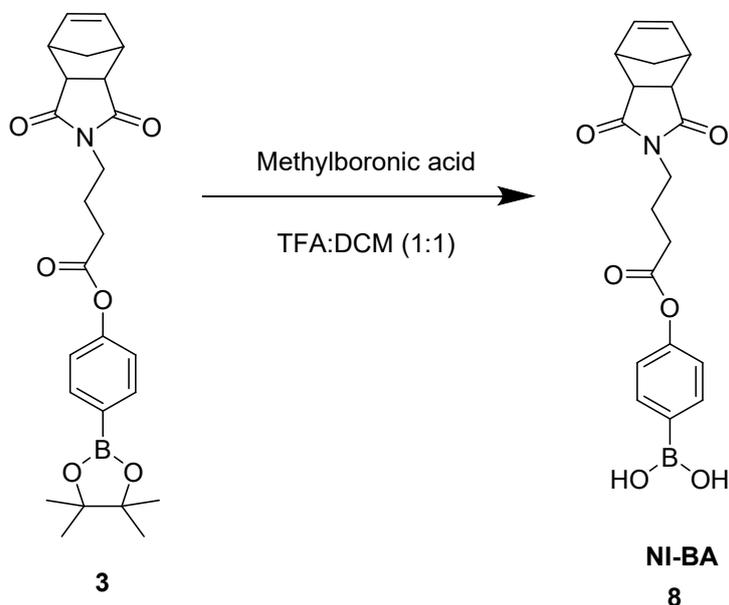
3 (250 mg, 0.55 mmol, eq) was taken in a 20 mL vial, and a 5 mL 1:1 mixture of TFA and DCM was added to it and stirred. Then (166 mg, 2.77 mmol, 5.0 eq) of methylboronic acid was added to the mixture and the reaction was allowed to run overnight. Afterwards, the solvent was completely evaporated and dried under vacuum to remove the methylboronic acid to yield **NI-BA** or **8**. 1H NMR (400 MHz, CDCl$_3$) 7.75 (d, 2H), 7.11 (d, 2H), 6.32 (t, 2H), 4.81 (s, 5H), 3.59 (t, 2H), 3.30 (t, 2H), 3.20 (s, 2H), 2.73 (s, 2H), 2.61 (t, 2H), 1.96 (m, 2H).
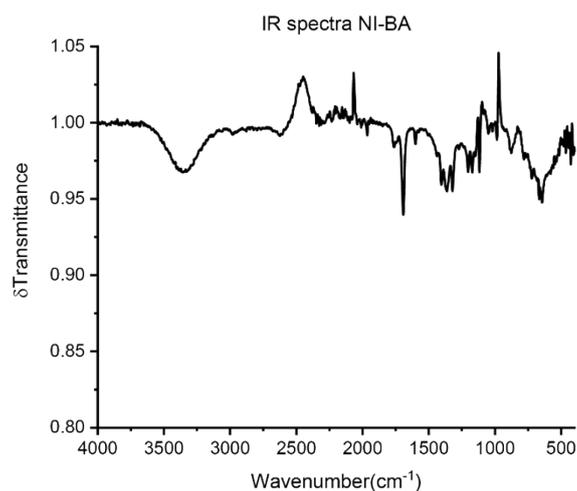
Figure S6. FT-IR spectra of NI-BA
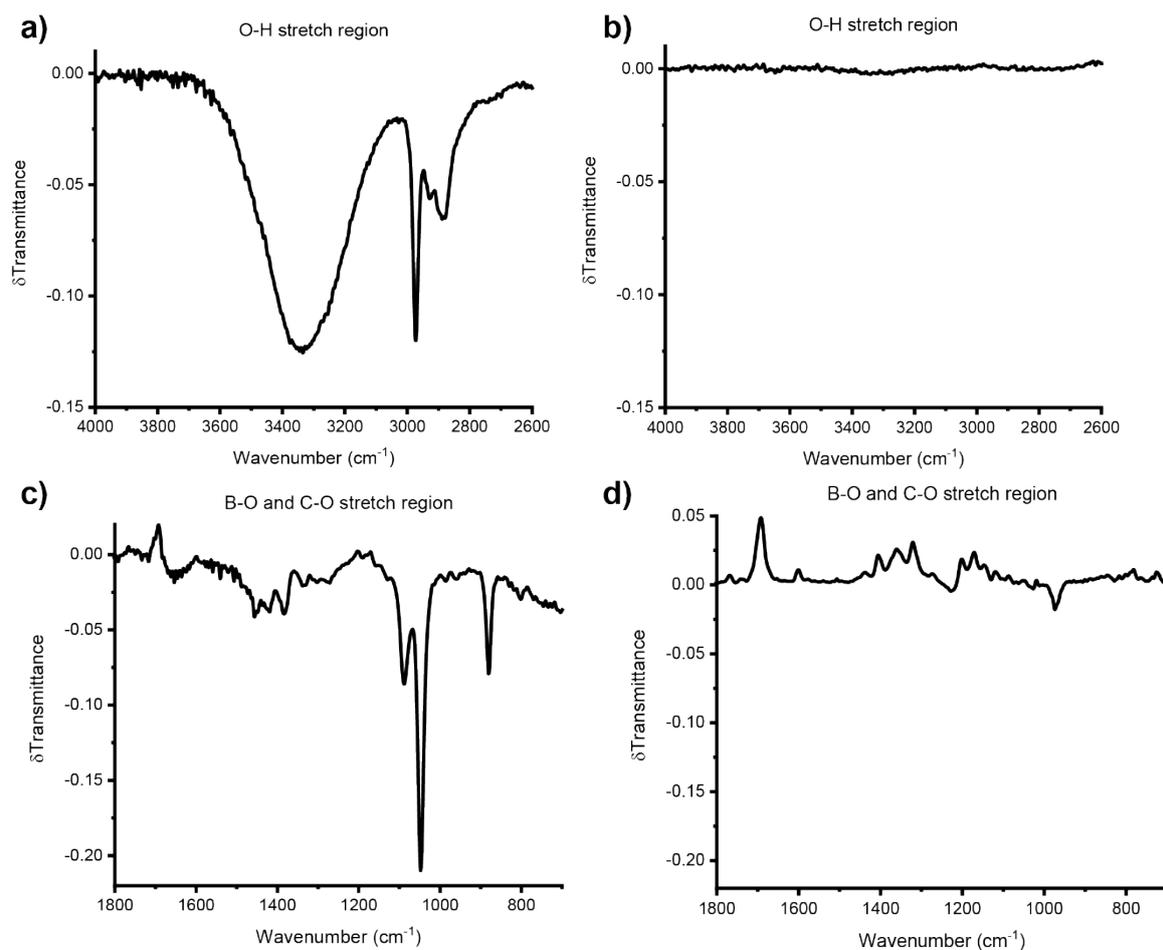
Figure S7. FTIR data for binding studies of **NI-BA** when interacting with saccharides. The difference spectra of **NI-BA** in the presence of a) 4 mg/mL of galactose and b) 4 mg/mL of mannose pentaacetate as control in the region of O-H stretching frequency to **NI-BA** only. The difference spectra of **NI-BA** in the presence of c) 4 mg/mL of galactose and d) 4 mg/mL mannose pentaacetate as control in the region of B-O and C-O stretching frequency.

3.3 pH-responsiveness of binding between boronic acid and diol
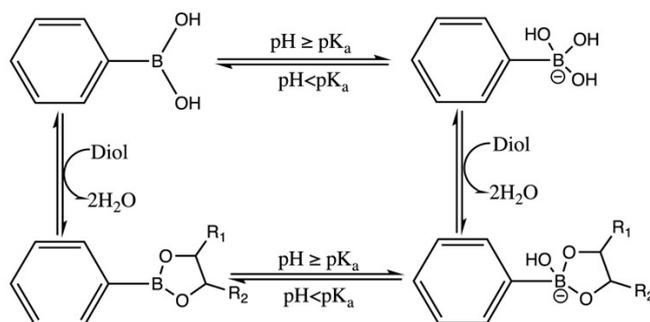
Scheme S1. The interaction between boronic acids and cis-diol-containing substances under different pH environment.

4. Sensing data

4.1 Sensing data for discrimination of cancer cell types

Table S1. Normalized fluorescence responses and LDA output for non-tumorigenic or tumorigenic cells. Score (1) and score (2) correspond to Figure 3 in the main text.

Sample name	I_{30}/I_0						LDA output	
	pH 5.8-Monomer	pH 5.8-Excimer	pH 7.4-Monomer	pH 7.4-Excimer	pH 8.2-Monomer	pH 8.2-Excimer	Score (1)	Score (2)
MCF10A	1.021	1.060	0.990	0.990	1.036	1.036	1.667	1.551
MCF10A	1.023	1.045	1.030	1.044	1.053	1.018	2.702	2.245
MCF10A	1.060	1.118	0.997	0.995	1.050	1.067	1.388	0.543
MCF10A	1.054	1.094	1.018	1.057	1.066	1.049	3.069	1.423
MCF10A	1.054	1.090	1.042	1.058	1.077	1.075	2.337	1.119
MCF10A	1.087	1.145	1.077	1.108	1.081	1.065	1.235	1.652
MCF-7	1.057	1.120	1.092	1.203	1.055	1.024	-1.028	5.359
MCF-7	1.042	1.064	1.082	1.173	1.029	0.991	0.139	6.64
MCF-7	1.044	1.091	1.065	1.153	1.014	0.950	-0.23	6.317
MCF-7	1.061	1.096	1.079	1.153	1.008	0.963	-0.628	6.867
MCF-7	1.067	1.106	1.076	1.139	1.024	0.949	0.983	5.459
MCF-7	1.099	1.152	1.091	1.167	1.044	1.001	0.385	4.906
HeLa	1.015	1.031	1.078	1.136	1.135	1.098	4.666	0.574
HeLa	1.037	1.061	1.038	1.050	1.109	1.079	4.946	-0.603
HeLa	1.007	1.012	1.049	1.051	1.098	1.037	5.294	0.366
HeLa	1.033	1.064	1.051	1.056	1.093	0.994	5.404	0.016
HeLa	1.024	1.046	1.063	1.069	1.120	1.043	5.779	-0.744
HeLa	1.043	1.076	1.078	1.096	1.159	1.121	5.547	-2.086
3T3	1.095	1.231	1.125	1.001	1.094	1.315	-10.933	-1.608
3T3	1.090	1.227	1.143	1.099	1.129	1.334	-9.695	1.055
3T3	1.117	1.259	1.116	1.030	1.068	1.262	-10.702	0.033
3T3	1.106	1.247	1.111	1.055	1.141	1.363	-8.297	-2.929
3T3	1.077	1.210	1.139	1.098	1.094	1.156	-6.895	0.115
3T3	1.074	1.209	1.207	1.035	1.122	1.249	-10.503	-2.255
4T1	1.055	1.142	0.997	1.006	1.187	1.298	3.033	-6.242
4T1	1.079	1.197	1.014	1.017	1.149	1.180	2.09	-5.041
4T1	1.121	1.245	0.984	0.979	1.174	1.265	3.163	-7.351
4T1	1.113	1.208	1.024	1.023	1.152	1.208	2.999	-4.628
4T1	1.110	1.268	1.042	1.060	1.188	1.255	0.32	-6.583
4T1	1.136	1.239	1.064	1.098	1.176	1.260	1.756	-4.062

Table S2. Percentage of accurate classification of cell types from Jackknifed analysis. The results show an overall 100% correct classification.

	3T3	4T1	HeLa	MCF10A	MCF-7	Correct (%)
3T3	6	0	0	0	0	100
4T1	0	6	0	0	0	100
HeLa	0	0	6	0	0	100
MCF10A	0	0	0	6	0	100
MCF-7	0	0	0	0	6	100
Total	6	6	6	6	6	100

Table S3. Prediction of unknown cell types using training set from Figure 3 and Table S1. The results show an overall 93% correct unknown identification.

Unknown sample #	I_{30}/I_0						True ID	Identified as	Correct prediction
	pH 5.8-Monomer	pH 5.8-Excimer	pH 7.4-Monomer	pH 7.4-Excimer	pH 8.2-Monomer	pH 8.2-Excimer			
1	1.022	1.034	1.003	0.999	0.999	1.034	MCF10A	MCF10A	Yes
2	1.013	1.059	1.001	0.988	0.997	0.953	MCF10A	MCF10A	Yes
3	1.000	0.984	0.980	0.978	1.028	0.995	MCF10A	MCF10A	Yes
4	1.008	1.006	1.005	1.010	1.033	1.007	MCF10A	MCF10A	Yes
5	1.053	1.076	0.957	0.961	1.042	1.019	MCF10A	MCF10A	Yes
6	1.052	1.097	0.970	0.991	1.075	1.050	MCF10A	MCF10A	Yes
7	1.054	1.135	1.058	1.136	1.146	1.139	MCF-7	HeLa	No
8	1.053	1.125	1.059	1.143	1.065	1.026	MCF-7	MCF-7	Yes
9	1.066	1.148	1.073	1.131	1.048	1.011	MCF-7	MCF-7	Yes
10	1.080	1.215	1.086	1.154	1.035	0.991	MCF-7	MCF-7	Yes
11	1.092	1.190	1.100	1.187	1.044	1.009	MCF-7	MCF-7	Yes
12	1.086	1.174	1.122	1.222	1.033	0.986	MCF-7	MCF-7	Yes
13	1.024	1.045	1.047	1.037	1.125	1.108	HeLa	HeLa	Yes
14	1.043	1.065	1.031	1.023	1.118	1.110	HeLa	HeLa	Yes
15	1.046	1.074	1.091	1.096	1.221	1.190	HeLa	HeLa	Yes
16	1.032	1.063	1.057	1.048	1.058	1.061	HeLa	MCF10A	No
17	1.066	1.102	1.046	1.020	1.167	1.170	HeLa	HeLa	Yes
18	1.056	1.127	1.095	1.096	1.171	1.005	HeLa	HeLa	Yes
19	1.094	1.252	1.157	1.088	1.114	1.363	3T3	3T3	Yes
20	1.094	1.243	1.155	1.098	1.077	1.270	3T3	3T3	Yes
21	1.062	1.158	1.151	1.052	1.110	1.308	3T3	3T3	Yes
22	1.057	1.178	1.159	1.028	1.074	1.283	3T3	3T3	Yes
23	1.077	1.222	1.192	1.091	1.106	1.309	3T3	3T3	Yes
24	1.082	1.236	1.155	1.028	1.083	1.168	3T3	3T3	Yes
25	1.037	1.113	1.016	1.002	1.120	1.204	4T1	4T1	Yes
26	1.043	1.118	1.005	0.967	1.141	1.198	4T1	4T1	Yes
27	1.030	1.084	0.994	0.966	1.129	1.190	4T1	4T1	Yes
28	1.025	1.112	1.013	0.992	1.130	1.211	4T1	4T1	Yes
29	1.067	1.186	1.012	1.024	1.150	1.251	4T1	4T1	Yes
30	1.083	1.231	1.038	1.057	1.173	1.235	4T1	4T1	Yes

4.2 Sensing data for identification of Chinese hamster ovary (CHO) mutated cells.

Table S4. Normalized fluorescence responses and LDA output for CHO cell lines. Score (1) and score (2) correspond to Figure 4 in the main text.

Sample name	I_{30}/I_0						LDA output	
	pH 5.8-Monomer	pH 5.8-Excimer	pH 7.4-Monomer	pH 7.4-Excimer	pH 8.2-Monomer	pH 8.2-Excimer	Score (1)	Score (2)
CRL-2241	1.018	1.118	0.903	1.040	0.893	1.075	-4.115	-2.443
CRL-2241	1.037	1.101	0.906	1.007	0.910	1.120	-3.739	-2.259
CRL-2241	1.016	1.101	0.889	1.014	0.886	1.102	-3.396	-3.486
CRL-2241	1.037	1.092	0.865	1.017	0.916	1.097	-4.353	-3.824
CRL-2241	1.048	1.083	0.855	0.993	0.889	1.065	-4.956	-3.792
CRL-2241	1.016	1.061	0.883	1.011	0.889	1.088	-3.928	-4.064
CRL-1735	1.130	1.183	0.928	1.189	0.982	1.175	3.110	-0.822
CRL-1735	1.082	1.159	0.938	1.170	0.962	1.214	4.230	-2.220
CRL-1735	1.128	1.192	0.880	1.144	0.929	1.190	4.799	-3.238
CRL-1735	1.092	1.189	0.910	1.255	0.978	1.228	7.437	-4.008
CRL-1735	1.042	1.149	0.905	1.152	0.836	1.105	4.431	-4.457
CRL-1735	1.044	1.120	0.925	1.149	0.880	1.139	3.887	-3.835
CRL-1736	1.204	1.229	1.006	1.241	1.019	1.244	6.971	3.159
CRL-1736	1.238	1.229	1.016	1.251	1.043	1.295	9.022	3.557
CRL-1736	1.244	1.252	1.014	1.292	1.009	1.244	10.007	3.623
CRL-1736	1.219	1.223	1.008	1.299	1.017	1.240	9.417	2.606
CRL-1736	1.226	1.252	0.979	1.217	1.021	1.288	8.256	2.399
CRL-1736	1.225	1.247	1.016	1.307	0.992	1.212	9.639	3.367
CRL-2242	1.050	1.085	0.893	1.101	0.903	1.079	-1.119	-3.614
CRL-2242	1.049	1.105	0.877	1.099	0.898	1.116	0.550	-4.675
CRL-2242	1.047	1.087	0.864	1.077	0.881	1.099	0.005	-5.240
CRL-2242	1.048	1.083	0.849	1.073	0.925	1.160	0.462	-6.151
CRL-2242	1.054	1.093	0.847	1.046	0.911	1.166	0.465	-5.911
CRL-2242	1.032	1.080	0.849	1.066	0.902	1.140	0.172	-6.390
CCL-61	1.069	1.107	0.972	1.029	0.949	1.011	-9.415	3.332
CCL-61	1.067	1.091	0.974	1.029	0.940	1.020	-8.492	2.839
CCL-61	1.128	1.101	0.960	1.014	0.937	0.993	-8.807	3.990
CCL-61	1.085	1.131	0.948	1.015	0.935	1.022	-8.486	2.689
CCL-61	1.073	1.087	0.927	1.005	0.926	0.990	-9.594	1.452
CCL-61	1.043	1.079	0.942	0.996	0.935	0.989	-11.013	1.772
CRL-2244	1.265	1.173	1.041	1.129	1.011	1.155	0.695	7.717
CRL-2244	1.219	1.178	1.041	1.158	1.024	1.175	1.035	6.539
CRL-2244	1.186	1.153	1.023	1.133	1.009	1.135	-1.272	5.598
CRL-2244	1.222	1.179	1.019	1.154	1.011	1.130	-0.250	6.203
CRL-2244	1.192	1.168	0.996	1.138	1.005	1.145	0.293	4.463
CRL-2244	1.189	1.158	1.007	1.128	0.997	1.120	-1.364	5.125

Table S5. Percentage of accurate classification of CHO glycosylation mutants from Jackknifed analysis. The results show an overall 100% correct classification.

	CCL-61	CRL-1735	CRL-1736	CRL-2241	CRL-2242	CRL-2244	Correct (%)
CCL-61	6	0	0	0	0	0	100
CRL-1735	0	6	0	0	0	0	100
CRL-1736	0	0	6	0	0	0	100
CRL-2241	0	0	0	6	0	0	100
CRL-2242	0	0	0	0	6	0	100
CRL-2244	0	0	0	0	0	6	100
Total	6	6	6	6	6	6	100

Table S6. Prediction of unknown cell types using training set from Figure 4 and Table S4. The results show an overall 100% correct unknown identification.

Unknown sample #	I_{30}/I_0						True ID	Identified as	Correct prediction
	pH 5.8-Monomer	pH 5.8-Excimer	pH 7.4-Monomer	pH 7.4-Excimer	pH 8.2-Monomer	pH 8.2-Excimer			
1	1.033	1.101	0.803	1.028	0.865	1.015	CRL-2241	CRL-2241	Yes
2	1.022	1.110	0.821	1.039	0.882	1.072	CRL-2241	CRL-2241	Yes
3	1.026	1.100	0.808	1.030	0.858	1.029	CRL-2241	CRL-2241	Yes
4	1.013	1.099	0.847	1.021	0.870	1.015	CRL-2241	CRL-2241	Yes
5	1.046	1.097	0.810	0.992	0.866	1.044	CRL-2241	CRL-2241	Yes
6	1.014	1.080	0.825	1.009	0.865	1.035	CRL-2241	CRL-2241	Yes
7	1.022	1.156	0.980	1.122	0.952	1.150	CRL-1735	CRL-1735	Yes
8	1.120	1.172	0.986	1.185	0.986	1.188	CRL-1735	CRL-1735	Yes
9	1.109	1.176	0.975	1.144	0.982	1.221	CRL-1735	CRL-1735	Yes
10	1.111	1.178	0.972	1.146	0.977	1.196	CRL-1735	CRL-1735	Yes
11	1.094	1.149	0.964	1.139	0.948	1.157	CRL-1735	CRL-1735	Yes
12	1.093	1.144	0.946	1.102	0.956	1.153	CRL-1735	CRL-1735	Yes
13	1.237	1.260	1.022	1.185	1.023	1.226	CRL-1736	CRL-1736	Yes
14	1.182	1.225	1.052	1.258	1.025	1.229	CRL-1736	CRL-1736	Yes
15	1.221	1.238	1.028	1.204	0.974	1.239	CRL-1736	CRL-1736	Yes
16	1.171	1.202	1.038	1.230	1.017	1.209	CRL-1736	CRL-1736	Yes
17	1.227	1.213	1.009	1.192	1.024	1.229	CRL-1736	CRL-1736	Yes
18	1.180	1.201	1.008	1.164	0.991	1.194	CRL-1736	CRL-1736	Yes
19	1.051	1.085	0.919	1.094	0.902	1.061	CRL-2242	CRL-2242	Yes
20	1.061	1.101	0.916	1.112	0.936	1.125	CRL-2242	CRL-2242	Yes
21	1.059	1.084	0.927	1.106	0.831	1.065	CRL-2242	CRL-2242	Yes
22	1.062	1.083	0.911	1.119	0.920	1.133	CRL-2242	CRL-2242	Yes
23	1.070	1.085	0.901	1.099	0.907	1.105	CRL-2242	CRL-2242	Yes
24	1.032	1.053	0.910	1.068	0.905	1.114	CRL-2242	CRL-2242	Yes
25	1.084	1.125	0.934	1.019	0.968	1.047	CCL-61	CCL-61	Yes
26	1.084	1.105	0.914	1.015	0.936	1.034	CCL-61	CCL-61	Yes

27	1.054	1.099	0.904	1.015	0.926	1.017	CCL-61	CCL-61	Yes
28	1.077	1.104	0.902	0.999	0.922	1.029	CCL-61	CCL-61	Yes
29	1.077	1.086	0.901	0.999	0.919	1.038	CCL-61	CCL-61	Yes
30	1.046	1.101	0.917	1.015	0.917	1.024	CCL-61	CCL-61	Yes
31	1.193	1.184	0.996	1.125	1.007	1.170	CRL-2244	CRL-2244	Yes
32	1.208	1.184	0.967	1.149	1.015	1.209	CRL-2244	CRL-2244	Yes
33	1.222	1.197	0.985	1.139	1.009	1.190	CRL-2244	CRL-2244	Yes
34	1.198	1.189	0.997	1.164	1.007	1.205	CRL-2244	CRL-2244	Yes
35	1.213	1.201	0.978	1.128	0.984	1.141	CRL-2244	CRL-2244	Yes
36	1.193	1.191	0.996	1.125	0.991	1.174	CRL-2244	CRL-2244	Yes

[1] R. F. Landis, C. H. Li, A. Gupta, Y. W. Lee, M. Yazdani, N. Ngernyuang, I. Altinbasak, S. Mansoor, M. A. S. Khichi, A. Sanyal, V. M. Rotello, *J. Am. Chem. Soc.* **2018**, *140*, 6176–6182.