

Triphenylamine-Boronic-Acid-based Theragnostic Biomaterial for Diabetes with Concurrent Fluorescence Sensing of Glucose and Microviscosity

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1. Characterization using ^1H , ^{13}C , and HRMS

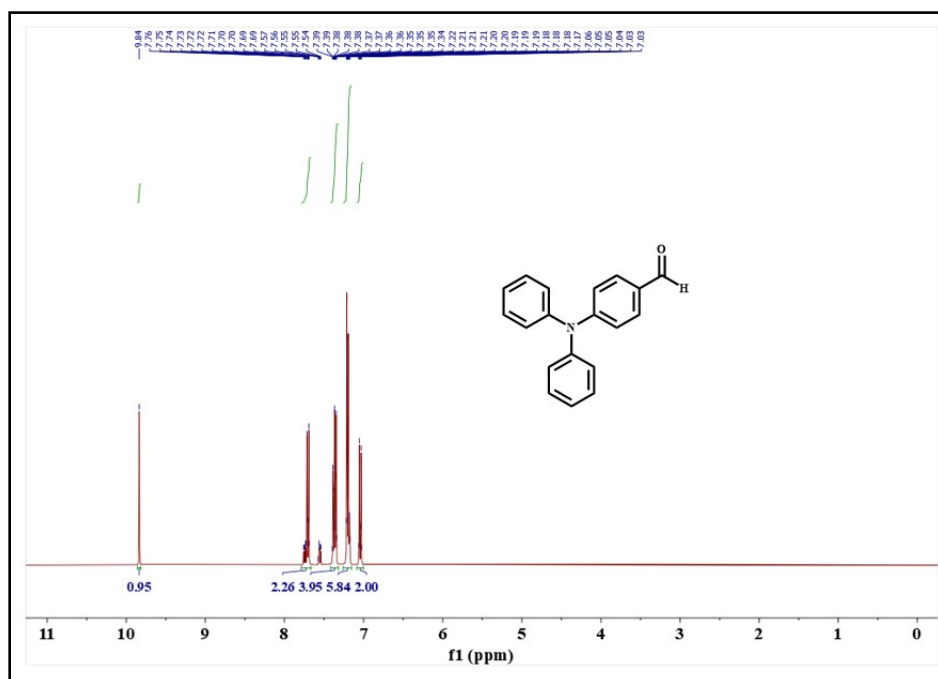


Figure S1. ^1H NMR (400 MHz, 298 K, CDCl_3) spectrum of 2

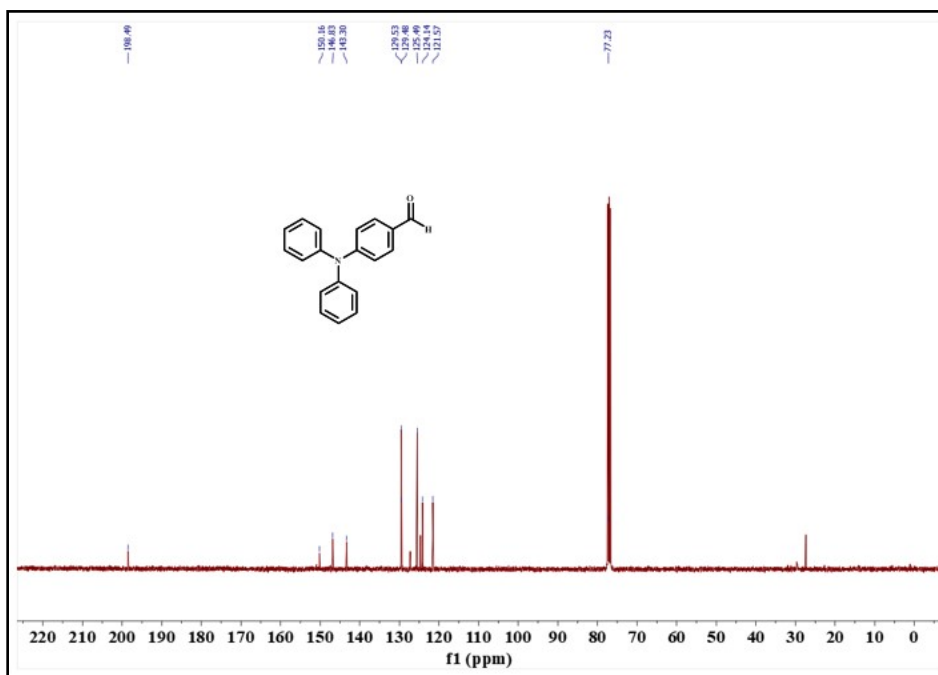


Figure S2. ^{13}C NMR (100 MHz, 298 K, CDCl_3) spectrum of 2

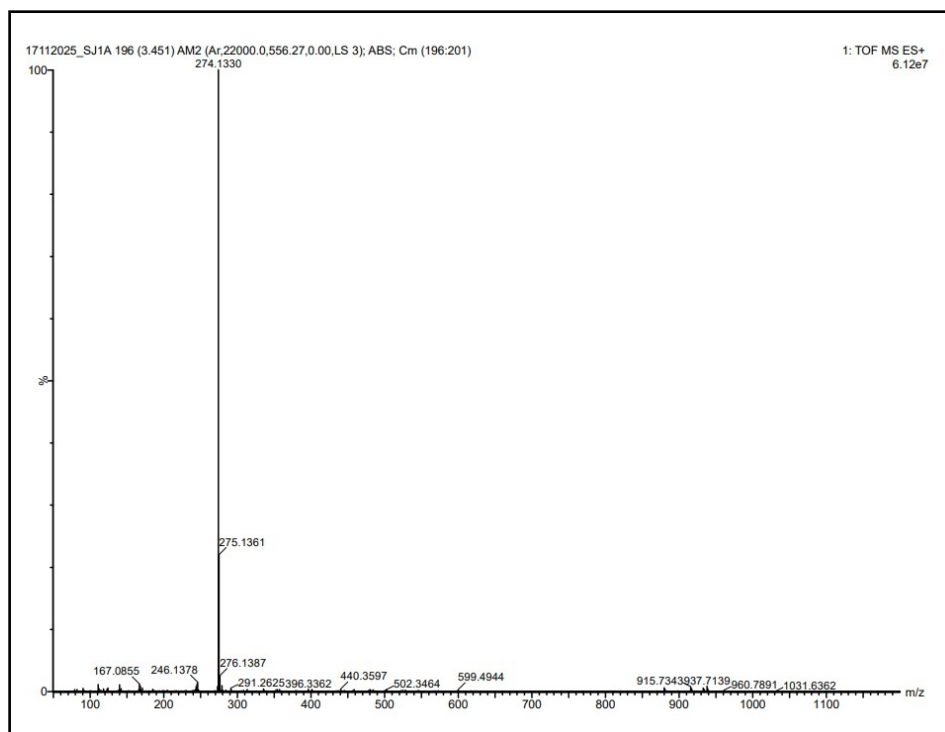


Figure S3. High-resolution mass spectrum of 2

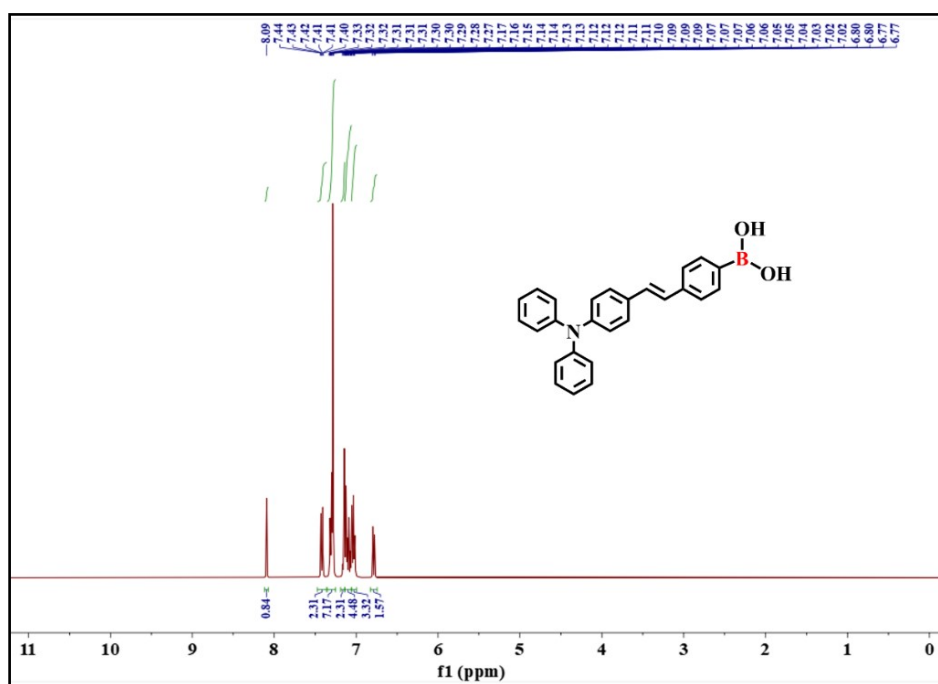


Figure S4. ^1H NMR (400 MHz, 298 K, CDCl_3) spectrum of 3a

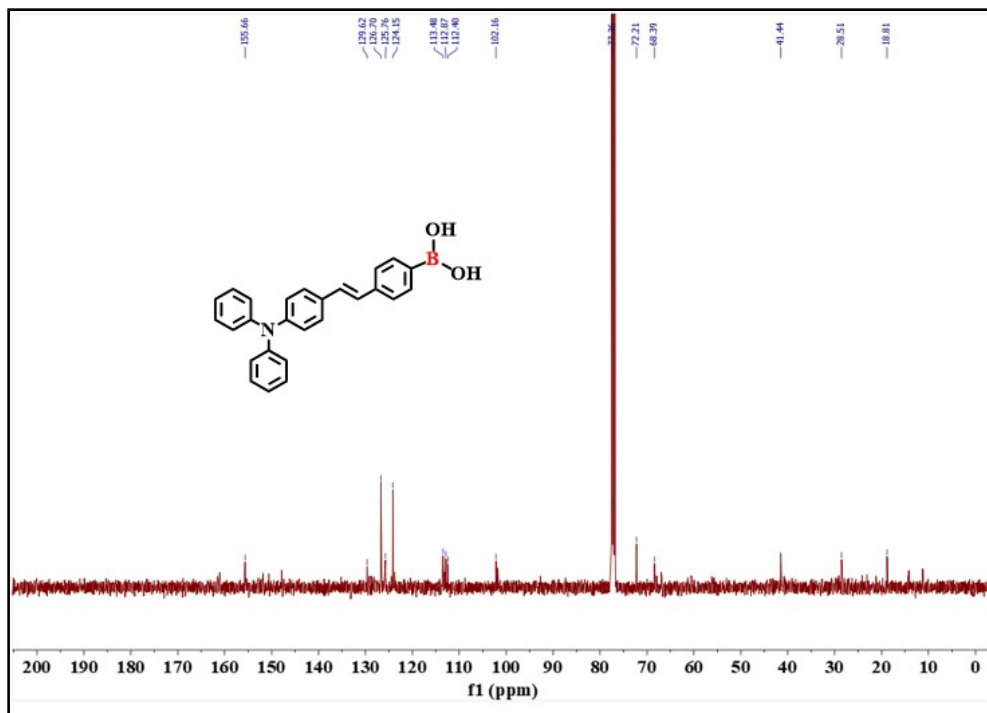


Figure S5. ¹³C NMR (100 MHz, 298 K, CDCl₃) spectrum of 3a

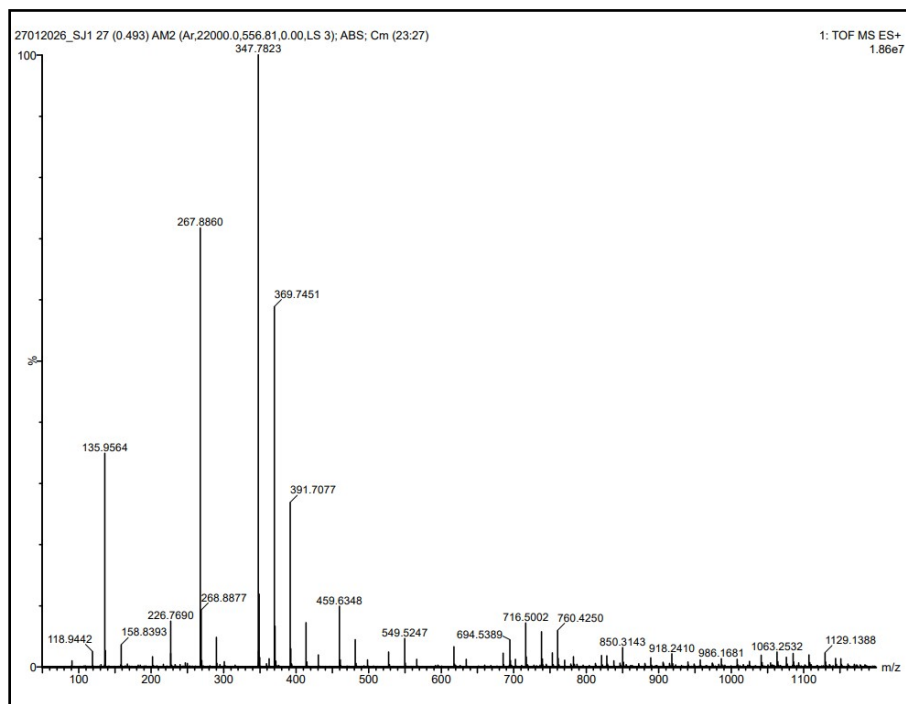


Figure S6. High-resolution mass spectrum of 3a

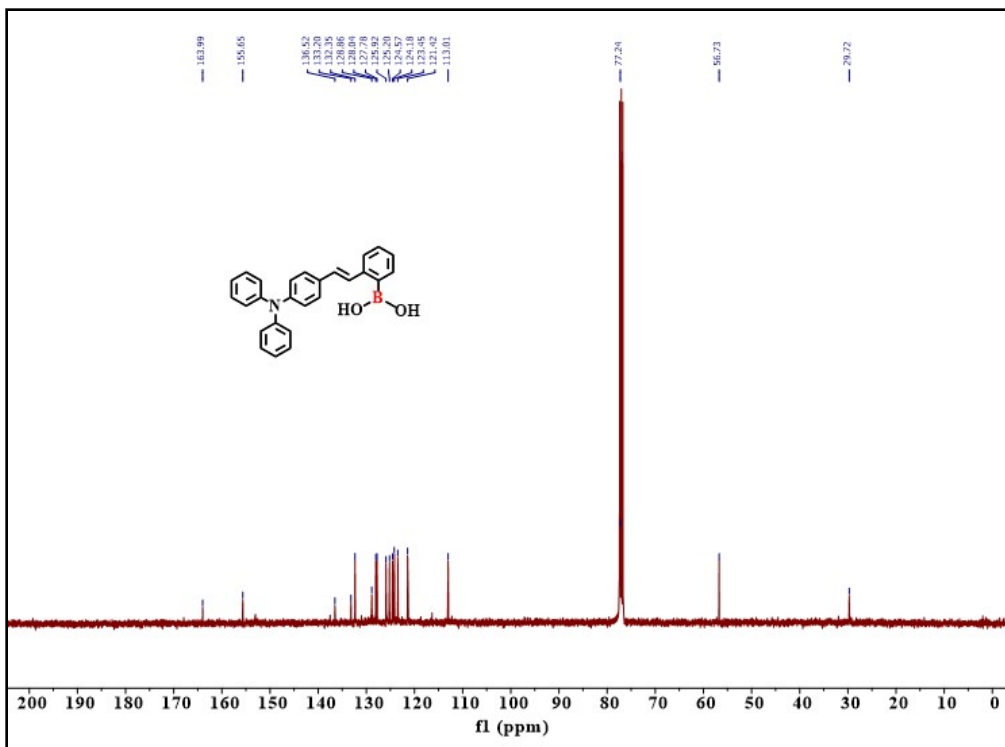


Figure S11. ¹³C NMR (100 MHz, 298 K, CDCl₃) spectrum of 3c

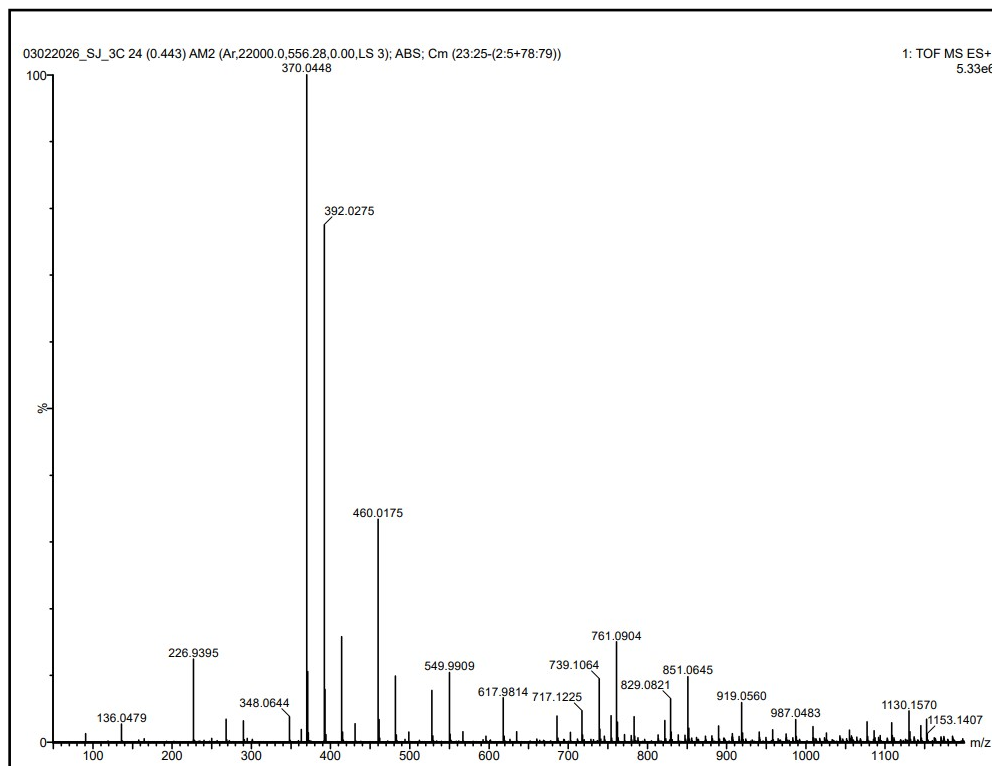


Figure S12. High-resolution mass spectrum of 3c

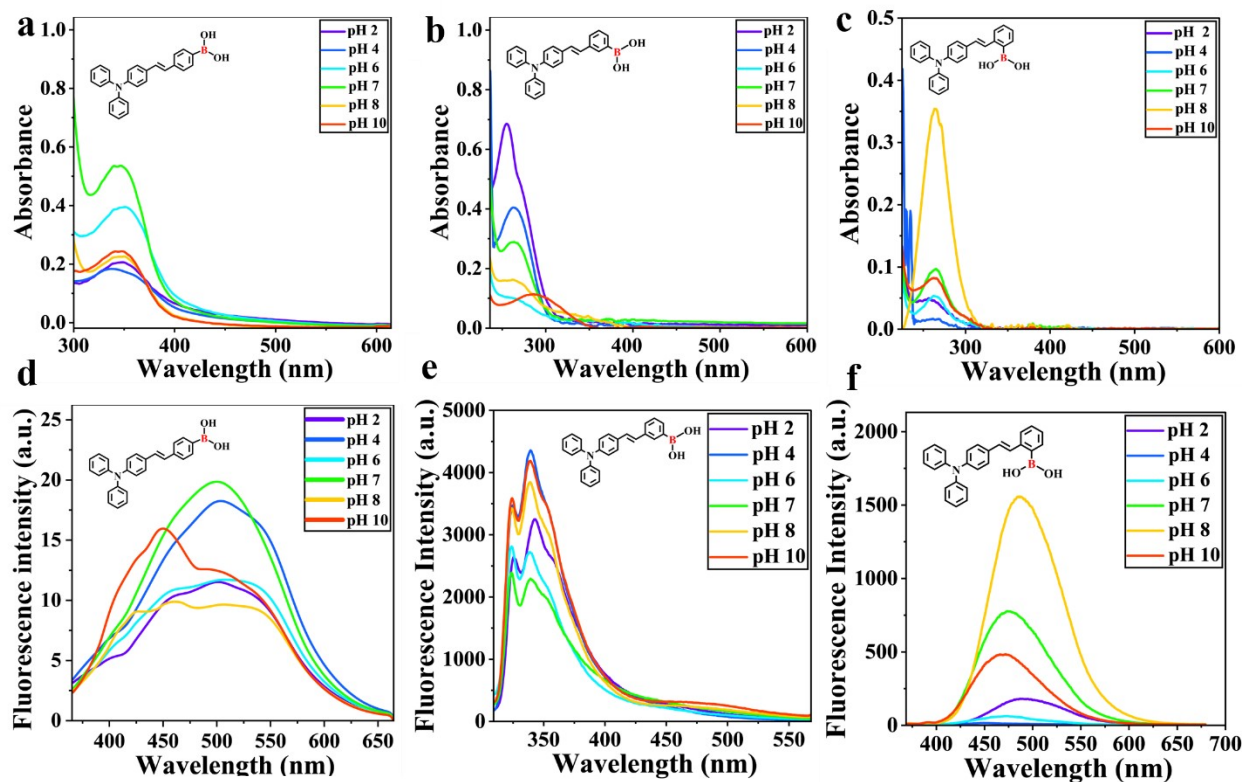


Figure S13. UV-Vis absorption spectra (a–c) and fluorescence emission spectra (d–f) of the compounds 3a, 3b, and 3c recorded at different pH levels (2–10). Sample concentration: (10 μ M)

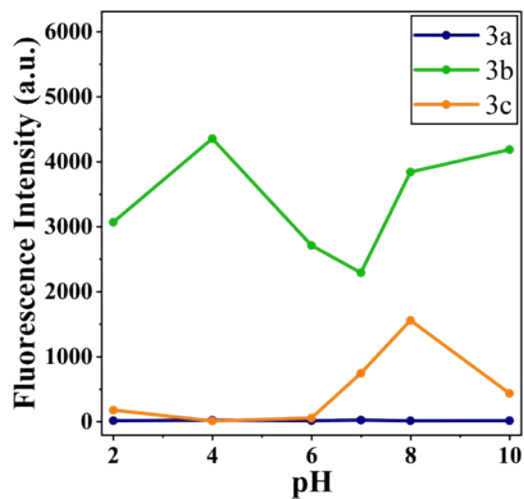


Figure S14 Stability studies of 3a, 3b, and 3c over physiological pH range. Sample concentration: 10 μ M.

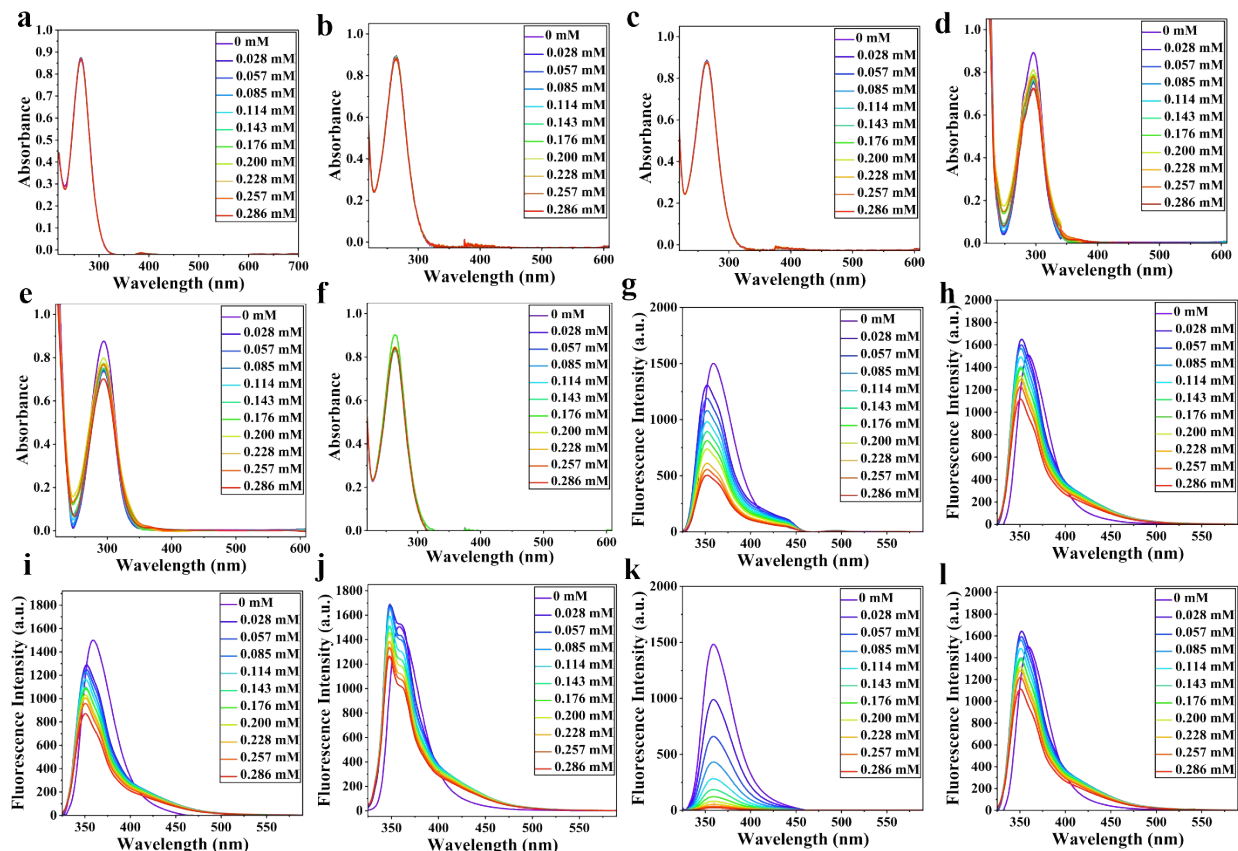


Figure S15. UV-Vis absorption spectra (a-f) and fluorescence emission spectra (g-l) for the titration of 3a with increasing concentrations of glucose (0 – 0.286 mM) in 2:8 ACN/PBS buffer at pH 2, 4, 6, 7, 8, and 10, respectively. Sample concentration: 10 μ M.

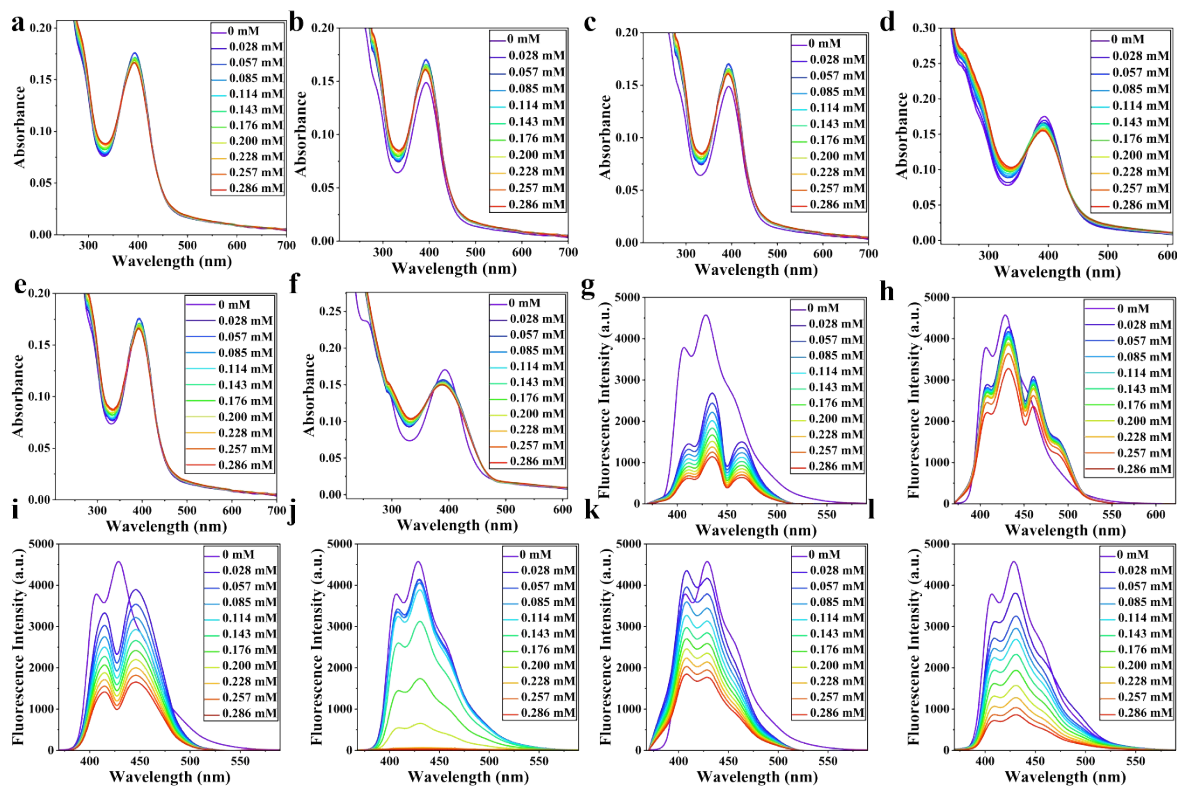


Figure S16. UV-Vis absorption spectra (a-f) and fluorescence emission spectra (g-l) for the titration of **3b** with increasing concentrations of glucose (0 – 0.286 mM) in 2:8 ACN/PBS buffer at pH 2, 4, 6, 7, 8, and 10, respectively. Sample concentration: 10 μM

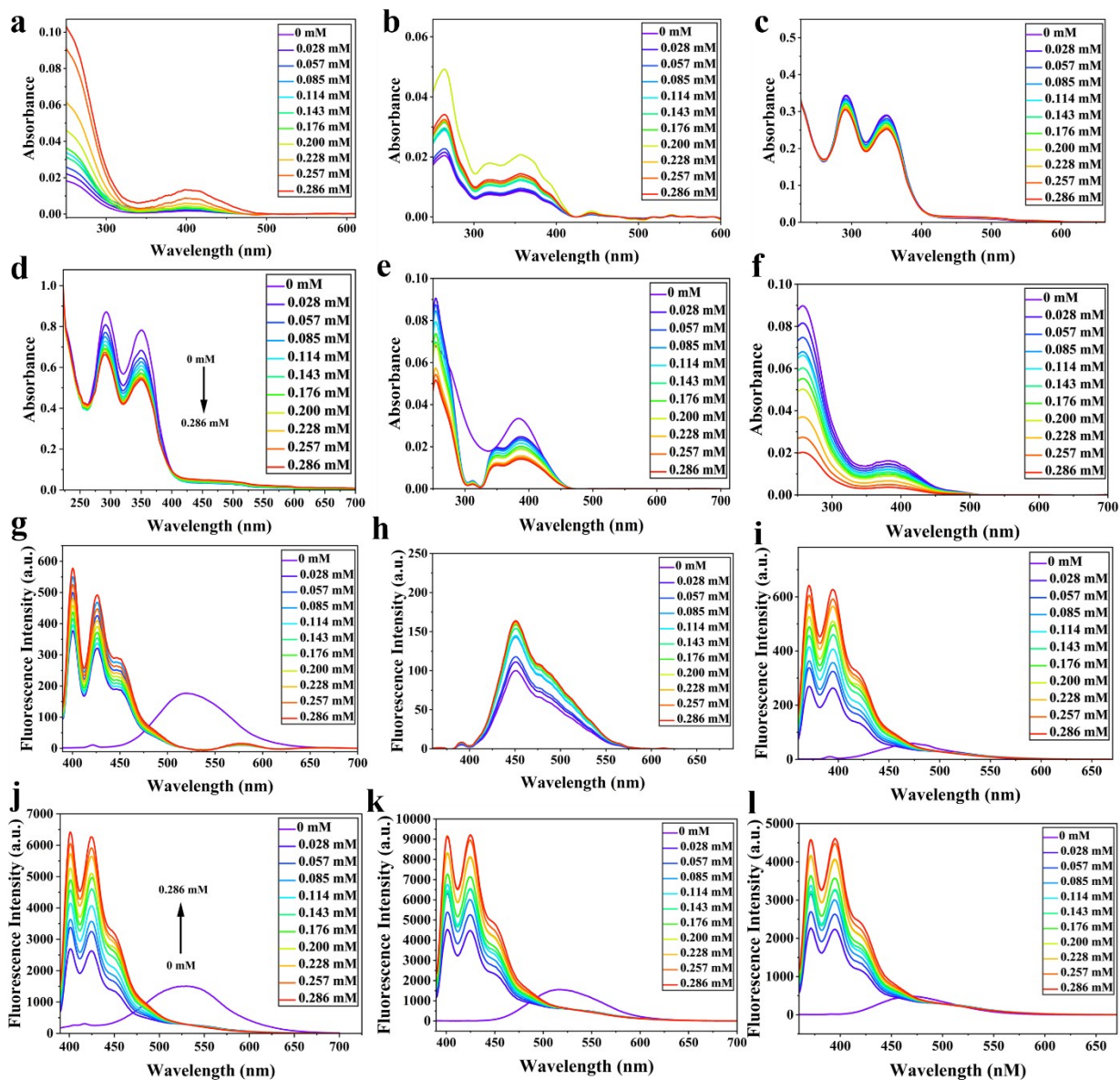


Figure S17. UV-Vis absorption spectra (a-f) and fluorescence emission spectra (g-l) for the titration of **3c** with increasing concentrations of glucose (0 – 0.286 mM) in 2:8 ACN/PBS buffer at pH 2, 4, 6, 7, 8, and 10, respectively. Sample concentration: 10 μ M

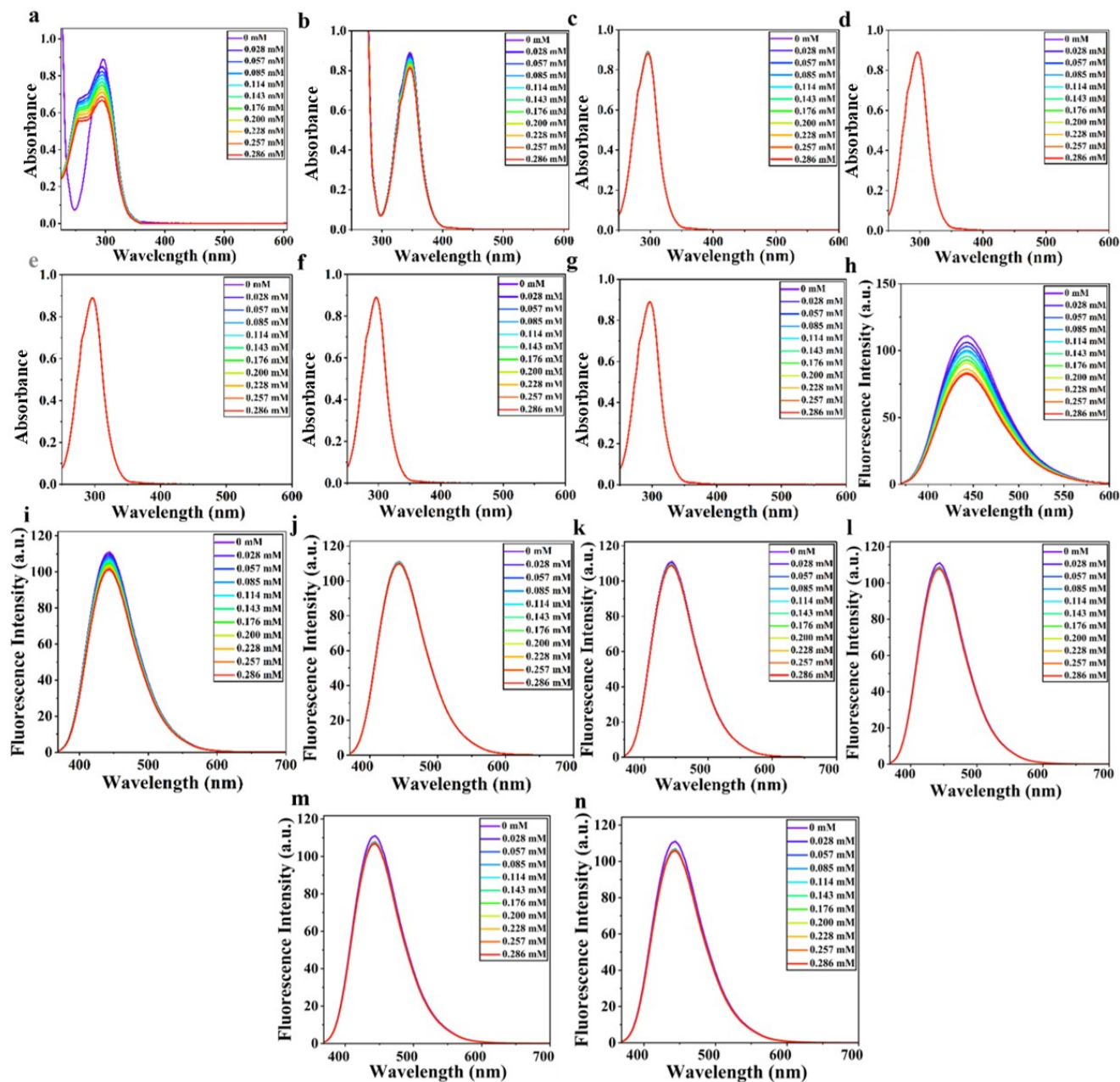


Figure S18. UV-Vis absorption spectra (a-g) and fluorescence emission spectra (h-n) of the compound **3a** in the presence of other competing saccharides (Fructose, Ribose, Mannose, Galactose, Maltose, Lactose, Sucrose). The sample solutions were maintained at 10 μ M in 2:8 ACN/PBS buffer (pH).

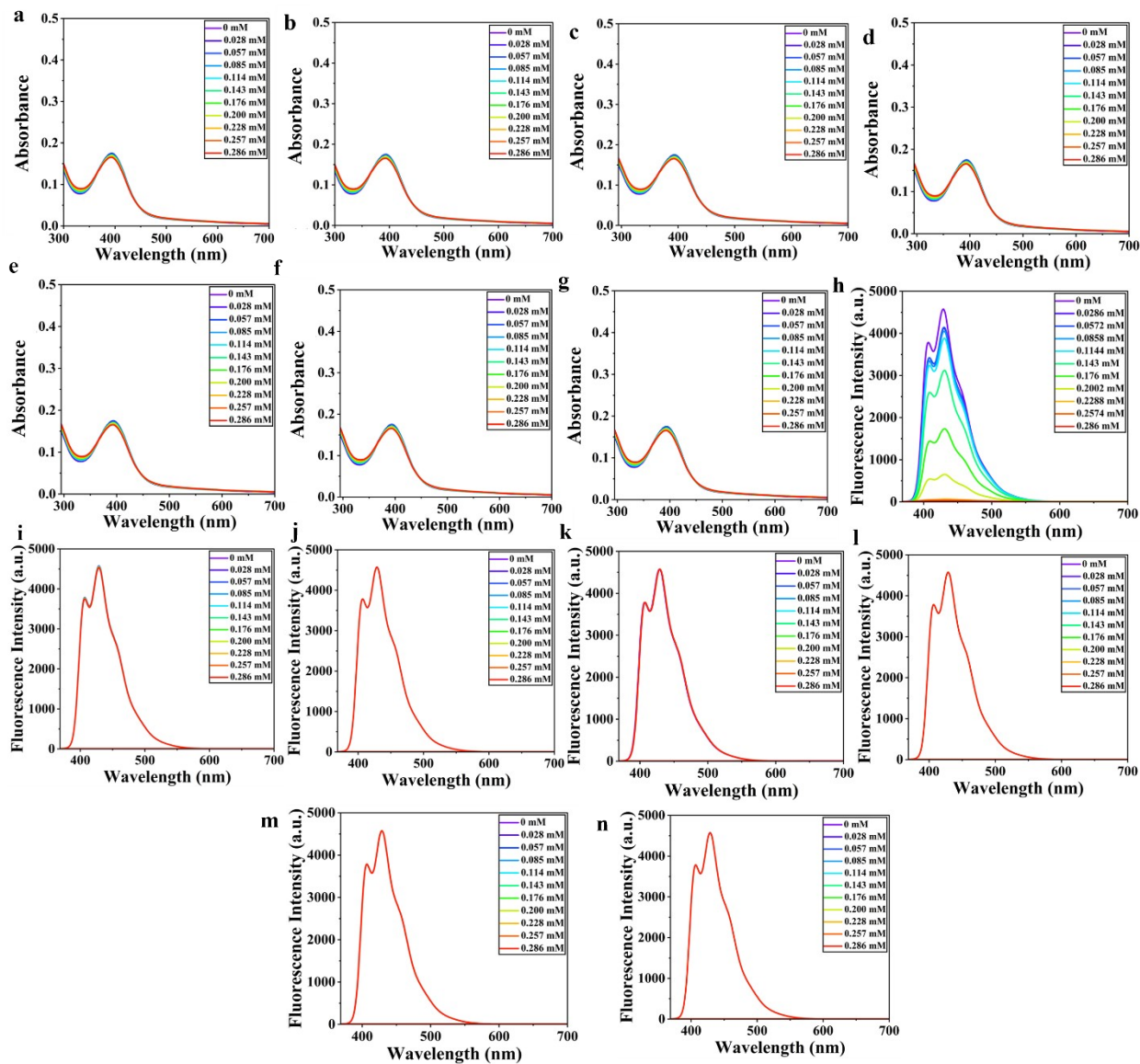


Figure S19. UV-Vis absorption spectra (a-g) and fluorescence emission spectra (h-n) of the compound **3b** in the presence of other competing saccharides (Fructose, Ribose, Mannose, Galactose, Maltose, Lactose, Sucrose). The sample solutions were maintained at 10 μ M in 2:8 ACN/PBS buffer (pH 7).

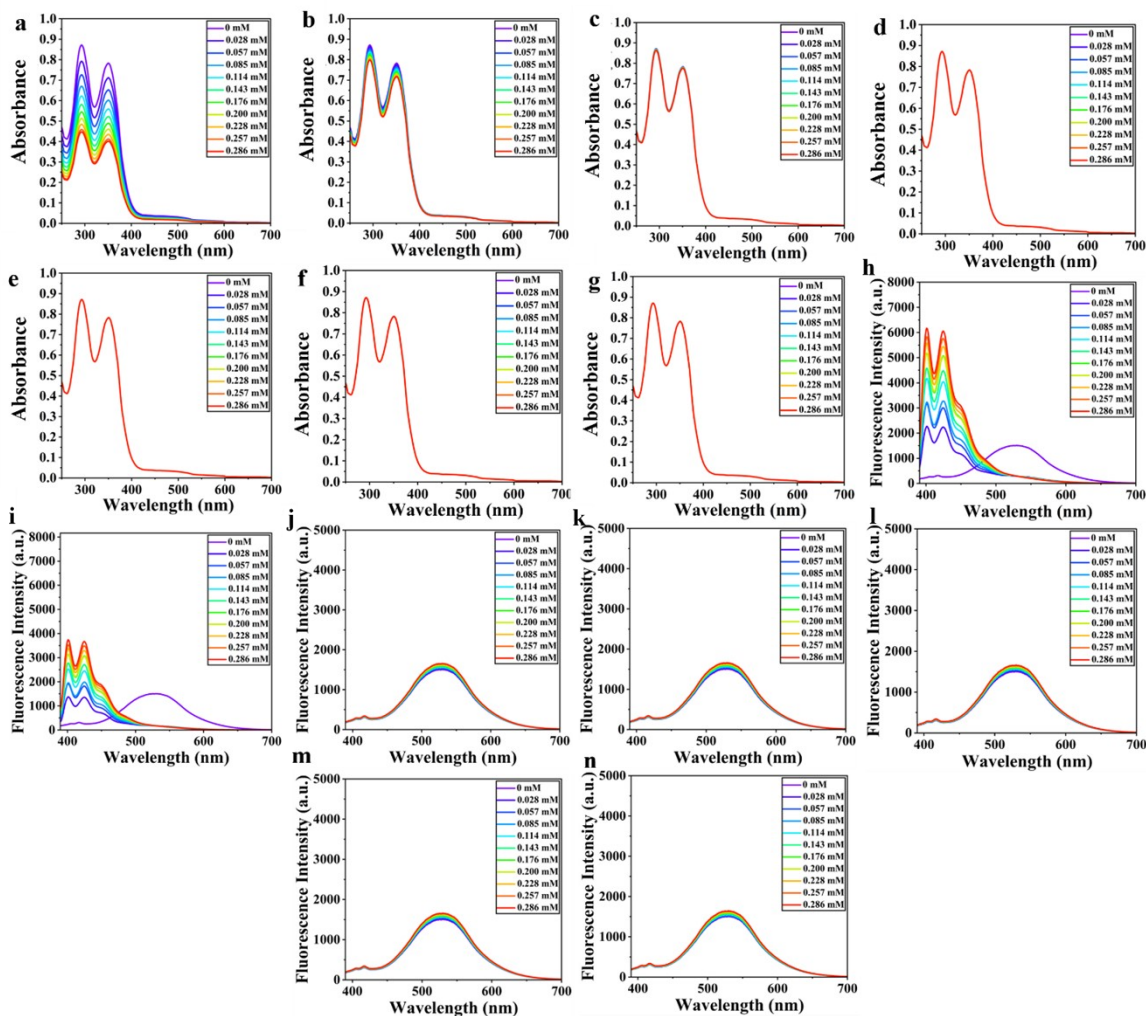


Figure S20. UV-Vis absorption spectra (a-g) and fluorescence emission spectra (h-n) of the compound **3c** in the presence of other competing saccharides (Fructose, Ribose, Mannose, Galactose, Maltose, Lactose, Sucrose). The sample solutions were maintained at 10 μ M in 2:8 ACN/PBS buffer (pH 7).

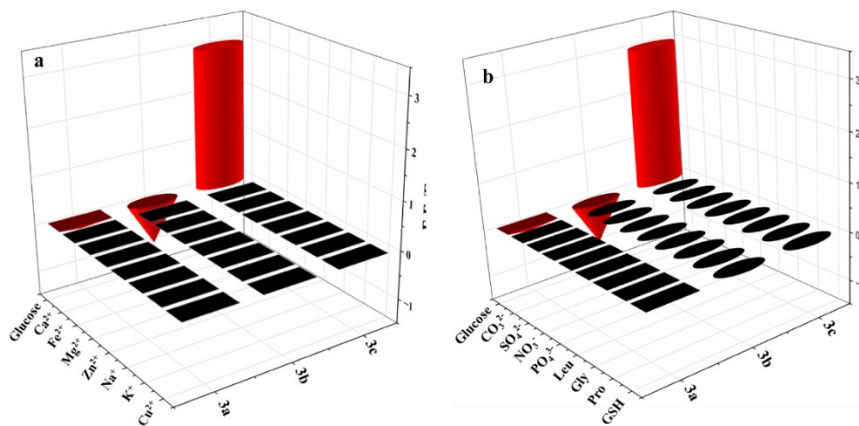


Figure 21. (a) Relative fluorescence response $(F - F_0)/F_0$ of probes **3a**, **3b**, and **3c**, respectively, in the presence of various metal ions. (b) Relative fluorescence response $(F - F_0)/F_0$ of probes **3a**, **3b**, and **3c**, respectively, in the presence of biologically relevant anions, amino acids, and GSH. [Leu: L-Leucine, Gly: L-Glycine, Pro: L-Proline, and GSH: Glutathione]

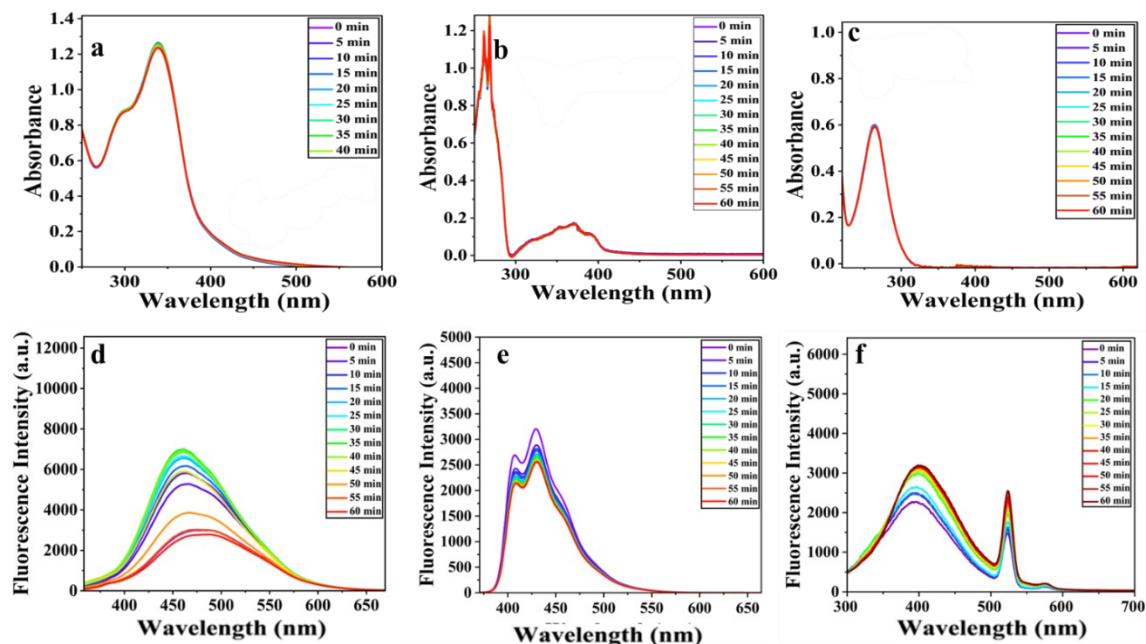


Figure S22. UV-Vis absorption spectra (a-c) and fluorescence emission spectra (d-f) of the compounds **3a**, **3b** and **3c** recorded at various time intervals from 0 to 60 minutes. Sample concentration: (10 μ M), solvent system: 2:8 ACN: PBS Buffer (pH 7)

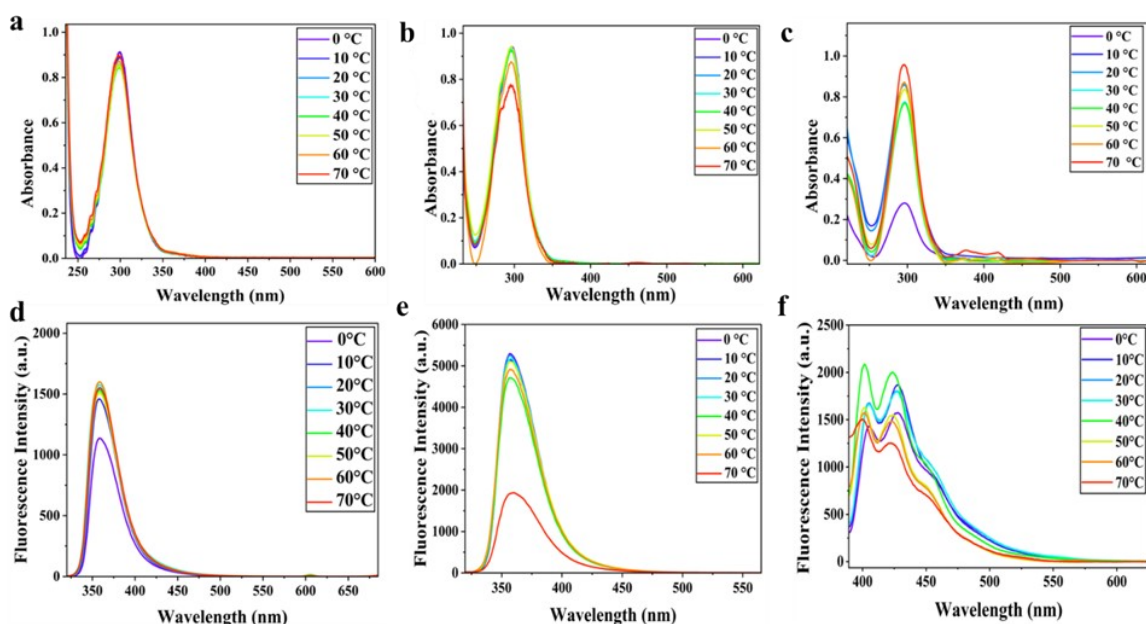


Figure S23. UV-Vis absorption spectra (a-c) and fluorescence emission spectra (d-f) of the compounds 3a, 3b and 3c recorded at various temperatures ranging from 0 to 70 °C. Sample concentration: (10 μM), solvent system: 2:8 ACN: PBS Buffer (pH 7).

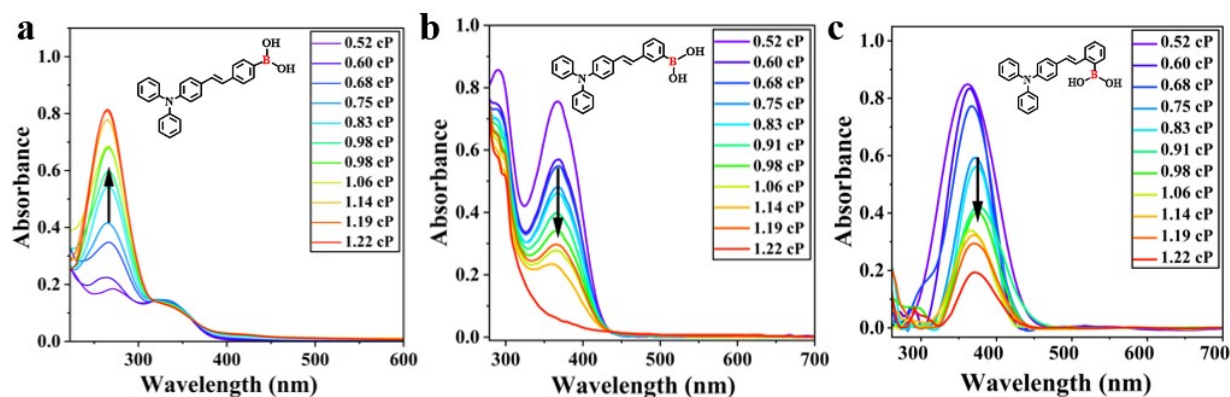


Figure S24. Absorbance spectra (a, b, c) of 3a, 3b, and 3c in solutions with varying viscosities (0.52–1.22 cP). Sample concentration: 10 μM. Solvent : THF.

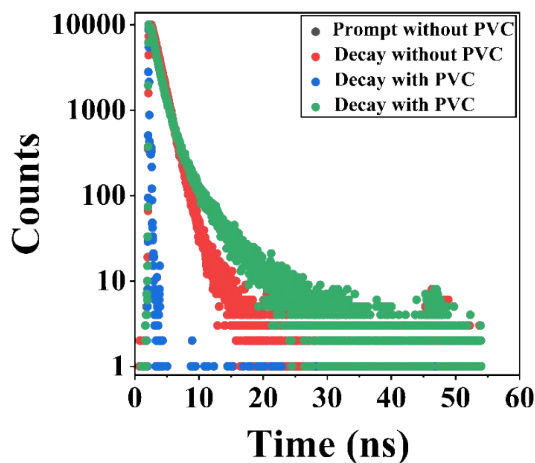


Figure S25. Fluorescence lifetime profile of 3c in the presence and absence of polyvinyl chloride (PVC).

Viscosity-responsiveness of TPA-TBA probes 3a-c in Glycerol-Water System

To render better physiological relevance, the TPA-TBA probes (**3a-c**) were pre-treated with constant amount of glucose (0.028 mM) and subjected to absorption and fluorescence experiments in presence of viscosity gradient solvent comprising of 0%–100% glycerol/water mixture. With increasing content of glycerol, a gradual increase in fluorescence intensity was observed (**Figure S26**). With increasing glycerol, the viscosity of the medium rises, which restricts the rotation across TPA units. Restricted molecular rotation inhibits non-radiative decay consequently enhancing the radiative fluorescence response. The increase in fluorescence for **3a-c** under high viscous medium with greater glycerol content further supported the viscosity-responsiveness of the probes under physiological conditions.

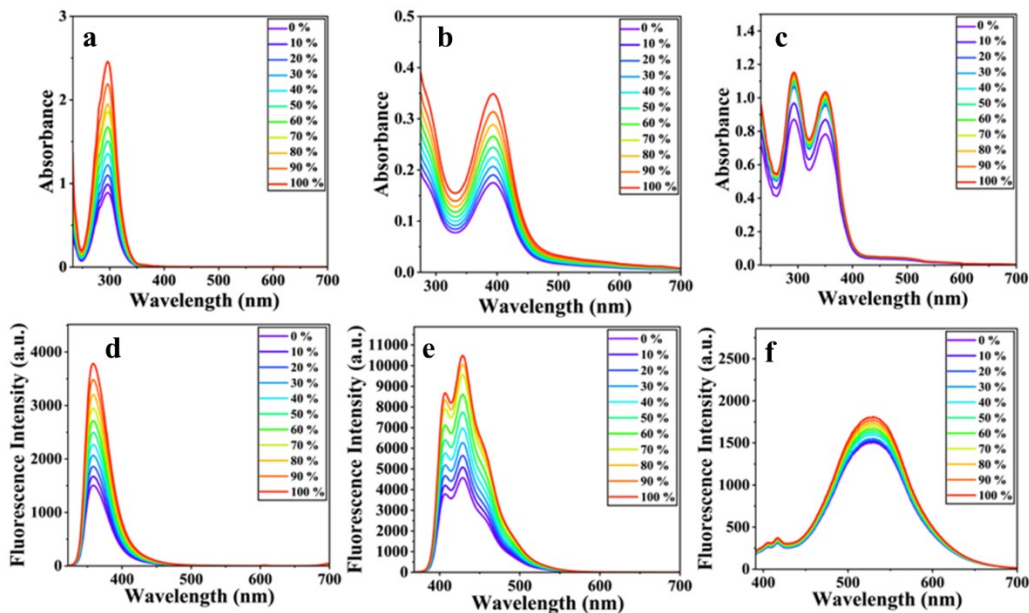


Figure S26. (a–c) Absorbance spectra and (d–f) fluorescence spectra of probes **3a**, **3b**, and **3c**, respectively, in water–glycerol mixtures with varying glycerol content (0–100%).

Electronic Excitation Analysis of Boronate Ester Complexes of TPA-TBA Probes with Glucose

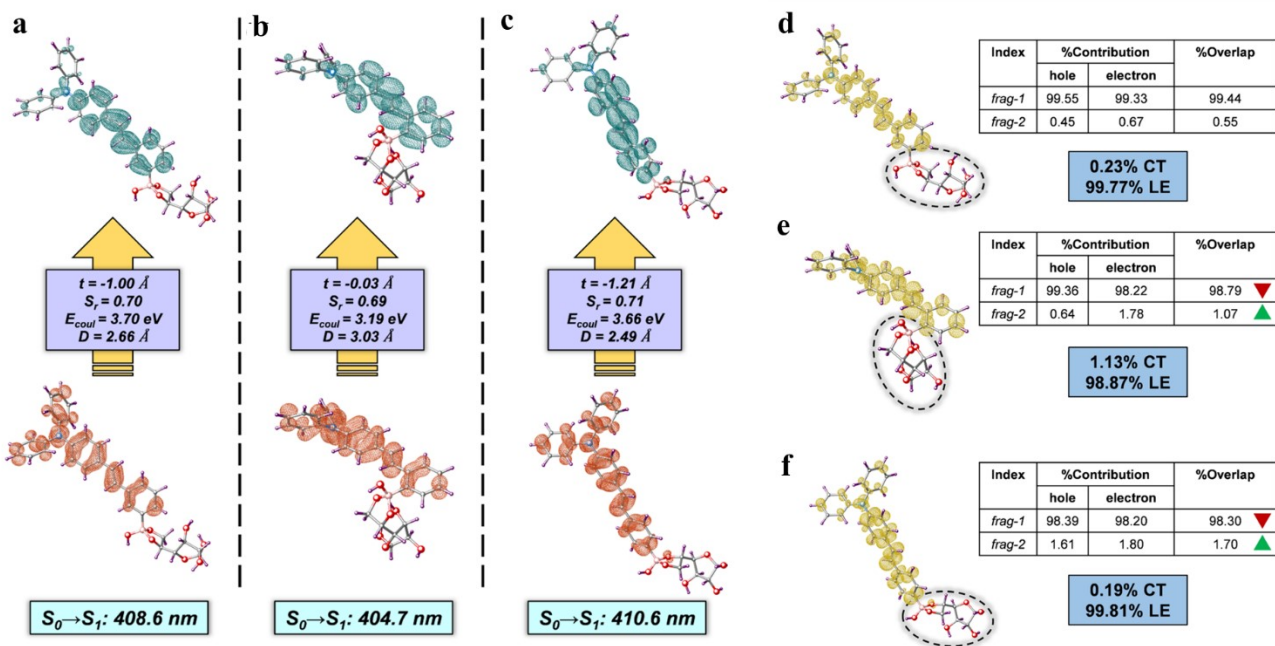


Figure S27 (a–f) Computed photophysical properties of boronate ester complexes of TPA-TBA probes with glucose using CPCM (2: 8 ACN/PBS)-TD-B3LYP-D4/def2-TZVP(-f)//B3LYP-D4/def2-SVP level of theory. The isosurfaces of the hole transition distribution (HTD) and the electron transition distribution (ETD) for the optically bright $S_0 \rightarrow S_1$ transition are shown in orange-red and dark cyan, respectively (isovalue = 0.001). Golden isosurfaces correspond to regions of hole-electron overlap. The hole-electron overlap (S_r), exciton binding energy (E_{coul}), overall estimate of the degree of spatial extension of HTD and ETD (H), and separation degree of hole and electron in the charge-transfer

(CT) direction (*t*) are shown. The real-space analyses of the electronic excitation of the TPA-TBA-glucose complexes are shown as follows: (a, d) meta, (b, e) ortho, and (c, f) para. Hole-electron %contributions, %overlap indices, and apparent charge-transfer (CT) and local excitation (LE) % contributions are shown in the corresponding tables. Grey-dotted areas denote the boron centre containing fragments (*frag-2*) used for the IFCT calculation.

Table S1. Binding constant of saccharides for 3a, 3b, 3c

| Compound | Glucose | Fructose | Ribose | Mannose | Galactose | Maltose | Lactose | Sucrose |
|-----------|--------------------------------------|----------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|
| 3a | 1.8×10^3 M ⁻¹ | 1.4×10^3 M ⁻¹ | 0.5×10^3 M ⁻¹ | 0.05×10^3 M ⁻¹ | 0.02×10^3 M ⁻¹ | 0.15×10^3 M ⁻¹ | 0.25×10^3 M ⁻¹ | 0.30×10^3 M ⁻¹ |
| 3b | 2.0×10^3 M ⁻¹ | 2.0×10^3 M ⁻¹ | 0.05×10^3 M ⁻¹ | 0.02×10^3 M ⁻¹ | 0.01×10^3 M ⁻¹ | 0.01×10^3 M ⁻¹ | 0.01×10^3 M ⁻¹ | 0.01×10^3 M ⁻¹ |
| 3c | 5.7×10^3 M ⁻¹ | 0.843×10^3 M ⁻¹ | 0.62×10^3 M ⁻¹ | 0.03×10^3 M ⁻¹ | 0.02×10^3 M ⁻¹ | 0.01×10^3 M ⁻¹ | 0.01×10^3 M ⁻¹ | 0.05×10^3 M ⁻¹ |

Table S2. Cartesian Coordinates of the DFT computed geometry for 3a

| In absence of Glucose | | | | | | | |
|------------------------------|-----------|----------|----------|---|-----------|----------|----------|
| | | | | C | -1.97756 | 0.08405 | 0.70338 |
| N | -7.61968 | 0.09564 | -0.05806 | C | -1.04222 | -0.61963 | 0.04455 |
| C | -8.28861 | -1.05000 | -0.55005 | C | 0.39797 | -0.56858 | 0.26367 |
| C | -9.30731 | -0.91837 | -1.49676 | C | 1.21948 | -1.48192 | -0.41156 |
| C | -9.97223 | -2.04114 | -1.96846 | C | 2.59430 | -1.47204 | -0.24037 |
| C | -9.62334 | -3.31005 | -1.51803 | C | 3.22182 | -0.54980 | 0.60367 |
| C | -8.60404 | -3.44338 | -0.58102 | B | 4.77037 | -0.50561 | 0.79925 |
| C | -7.94529 | -2.32419 | -0.09208 | O | 5.63531 | -1.45201 | 0.30438 |
| C | -8.36838 | 1.25419 | 0.26107 | O | 5.31422 | 0.53352 | 1.50203 |
| C | -9.58587 | 1.14367 | 0.93617 | C | 2.39503 | 0.36720 | 1.27233 |
| C | -10.32322 | 2.27974 | 1.23894 | C | 1.02245 | 0.36099 | 1.11115 |
| C | -9.85294 | 3.54081 | 0.88850 | C | -4.26017 | 0.74471 | 1.35988 |
| C | -8.63765 | 3.65279 | 0.22088 | C | -5.63456 | 0.75146 | 1.20043 |
| C | -7.90238 | 2.52052 | -0.09961 | H | -9.57487 | 0.06665 | -1.85423 |
| C | -6.22507 | 0.08026 | 0.12633 | H | -10.75935 | -1.92338 | -2.70248 |
| C | -5.39163 | -0.60014 | -0.77239 | H | -10.13974 | -4.18415 | -1.89212 |
| C | -4.02281 | -0.61265 | -0.59571 | H | -8.32806 | -4.42452 | -0.21579 |
| C | -3.41472 | 0.05865 | 0.47715 | H | -7.16102 | -2.42980 | 0.64510 |

| | | | | | | | |
|---|-----------|----------|----------|---|----------|----------|----------|
| H | -9.94987 | 0.16461 | 1.21668 | H | 0.76447 | -2.20519 | -1.07809 |
| H | -11.26475 | 2.17805 | 1.76372 | H | 3.18179 | -2.19609 | -0.79661 |
| H | -10.42647 | 4.42545 | 1.13186 | H | 5.20549 | -2.18476 | -0.14450 |
| H | -8.26412 | 4.62778 | -0.06559 | H | 6.27212 | 0.46061 | 1.57839 |
| H | -6.96243 | 2.60974 | -0.62717 | H | 2.85151 | 1.10035 | 1.92497 |
| H | -5.83063 | -1.11260 | -1.61738 | H | 0.42702 | 1.09660 | 1.63562 |
| H | -3.41216 | -1.13140 | -1.32286 | H | -3.82558 | 1.27096 | 2.20162 |
| H | -1.66210 | 0.74561 | 1.50385 | H | -6.25882 | 1.28152 | 1.90627 |
| H | -1.35619 | -1.31471 | -0.72746 | | | | |

In the presence of glucose

| | | | | | | | |
|---|----------|----------|----------|---|-----------|----------|----------|
| N | -7.16490 | 0.31320 | -0.01188 | C | 1.47750 | -2.18618 | -0.78161 |
| C | -7.97104 | -0.84864 | -0.00336 | C | 2.86210 | -2.33239 | -0.67622 |
| C | -9.10227 | -0.94015 | -0.83432 | C | 3.64642 | -1.49161 | 0.13608 |
| C | -9.89670 | -2.08727 | -0.81874 | B | 5.27995 | -1.62018 | 0.19759 |
| C | -9.57116 | -3.16844 | 0.00808 | O | 5.73195 | -2.99605 | -0.00419 |
| C | -8.44101 | -3.08350 | 0.82879 | C | 2.94795 | -0.49229 | 0.84656 |
| C | -7.65094 | -1.93310 | 0.83292 | C | 1.56716 | -0.33066 | 0.75230 |
| C | -7.76163 | 1.59376 | -0.07416 | C | -3.62348 | 0.92040 | 0.97199 |
| C | -8.93527 | 1.87313 | 0.64872 | C | -5.00821 | 1.04679 | 0.89926 |
| C | -9.52056 | 3.13815 | 0.58009 | H | -9.35449 | -0.10728 | -1.49340 |
| C | -8.94032 | 4.15075 | -0.19191 | H | -10.77232 | -2.14124 | -1.47154 |
| C | -7.76792 | 3.87759 | -0.90567 | H | -10.19116 | -4.06828 | 0.01192 |
| C | -7.18554 | 2.61044 | -0.85666 | H | -8.17587 | -3.91690 | 1.48515 |
| C | -5.75670 | 0.19376 | 0.07263 | H | -6.77871 | -1.86917 | 1.48604 |
| C | -5.07443 | -0.78676 | -0.67221 | H | -9.38529 | 1.09331 | 1.26581 |
| C | -3.69401 | -0.91687 | -0.58092 | H | -10.43263 | 3.33759 | 1.14938 |
| C | -2.92521 | -0.06671 | 0.24515 | H | -9.39709 | 5.14246 | -0.23653 |
| C | -1.47194 | -0.16259 | 0.38274 | H | -7.30625 | 4.65582 | -1.51955 |
| C | -0.65917 | -1.06861 | -0.20987 | H | -6.27810 | 2.40042 | -1.42588 |
| C | 0.79320 | -1.17849 | -0.07030 | H | -5.64005 | -1.45173 | -1.32813 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| H | -3.20158 | -1.68810 | -1.17732 | C | 6.53803 | 0.31210 | -0.24096 |
| H | -1.02901 | 0.58774 | 1.04627 | H | 7.24166 | 0.92207 | -2.14142 |
| H | -1.10605 | -1.81939 | -0.87170 | H | 9.86642 | 2.99654 | -0.76697 |
| H | 0.90219 | -2.86210 | -1.42374 | O | 9.13007 | 3.09508 | 1.08045 |
| H | 3.35730 | -3.13110 | -1.23866 | H | 9.92687 | -1.46853 | -0.89314 |
| H | 5.18136 | -3.58467 | 0.52667 | H | 11.48001 | 1.20565 | -0.88126 |
| H | 3.52015 | 0.16800 | 1.50479 | H | 8.58253 | 2.58506 | 1.69895 |
| H | 1.07878 | 0.45918 | 1.33032 | C | 6.85947 | -0.19429 | 1.17549 |
| H | -3.06076 | 1.59407 | 1.62466 | O | 5.92947 | -0.78490 | -0.85805 |
| H | -5.51795 | 1.81190 | 1.48815 | H | 5.81867 | 1.15950 | -0.13458 |
| C | 7.65280 | 0.88934 | -1.11909 | H | 7.80839 | -0.76713 | 1.17254 |
| C | 9.04059 | 0.22531 | -1.12224 | O | 5.76311 | -1.00999 | 1.48040 |
| C | 9.76647 | 0.95892 | 0.00324 | H | 6.96137 | 0.63269 | 1.90632 |
| H | 9.54475 | 0.52144 | -2.06935 | | | | |
| O | 9.01060 | -1.17200 | -1.00002 | | | | |
| C | 9.21022 | 2.38721 | -0.11524 | | | | |
| O | 11.17095 | 0.85209 | -0.03269 | | | | |
| H | 9.45677 | 0.53855 | 0.97341 | | | | |
| O | 7.93432 | 2.24767 | -0.71812 | | | | |

Table S3. Cartesian Coordinates of the DFT computed geometry for 3b

In absence of Glucose

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| N | -2.75699 | 7.05516 | 0.83367 | C | -2.15713 | 11.11586 | 1.78396 |
| C | -4.04541 | 6.60567 | 0.46260 | C | -1.21170 | 10.42127 | 1.03629 |
| C | -4.84253 | 7.37203 | -0.39165 | C | -1.40902 | 9.08608 | 0.71492 |
| C | -6.10976 | 6.93307 | -0.74697 | C | -1.68568 | 6.14248 | 0.91338 |
| C | -6.59706 | 5.71989 | -0.27206 | C | -1.55478 | 5.11216 | -0.02708 |
| C | -5.80221 | 4.95224 | 0.57261 | C | -0.51198 | 4.21076 | 0.05256 |
| C | -4.54042 | 5.39202 | 0.94645 | C | 0.45821 | 4.29852 | 1.06348 |
| C | -2.55528 | 8.41817 | 1.15334 | C | 1.57618 | 3.37346 | 1.19232 |
| C | -3.50025 | 9.11532 | 1.91018 | C | 1.77406 | 2.24389 | 0.49445 |
| C | -3.30312 | 10.45504 | 2.21346 | C | 2.90013 | 1.32322 | 0.62178 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 2.85449 | 0.09825 | -0.05404 | H | -2.00313 | 12.15873 | 2.02780 |
| C | 3.88640 | -0.84052 | 0.02696 | H | -0.31891 | 10.92509 | 0.68783 |
| C | 5.00239 | -0.52979 | 0.81140 | H | -0.67680 | 8.55124 | 0.12549 |
| B | 3.79853 | -2.19728 | -0.73722 | H | -2.28023 | 5.02824 | -0.82478 |
| O | 2.66917 | -2.46235 | -1.47239 | H | -0.43604 | 3.43906 | -0.70199 |
| O | 4.85788 | -3.06531 | -0.63720 | H | 2.29940 | 3.64920 | 1.95336 |
| C | 5.07438 | 0.68480 | 1.48524 | H | 1.02974 | 1.94174 | -0.23530 |
| C | 4.04016 | 1.60149 | 1.39107 | H | 1.98459 | -0.13073 | -0.65835 |
| C | 0.32370 | 5.34571 | 1.98507 | H | 5.81541 | -1.24010 | 0.88692 |
| C | -0.72716 | 6.24485 | 1.92382 | H | 2.65187 | -3.30552 | -1.93411 |
| H | -4.46366 | 8.31146 | -0.77067 | H | 4.77316 | -3.89517 | -1.11529 |
| H | -6.71452 | 7.53824 | -1.41056 | H | 5.94603 | 0.92102 | 2.08317 |
| H | -7.58315 | 5.37722 | -0.55657 | H | 4.12371 | 2.54751 | 1.90990 |
| H | -6.17120 | 4.00956 | 0.95667 | H | 1.05341 | 5.44274 | 2.78040 |
| H | -3.92965 | 4.79717 | 1.61171 | H | -0.80851 | 7.03341 | 2.65917 |
| H | -4.38814 | 8.60204 | 2.25326 | | | | |
| H | -4.04455 | 10.98110 | 2.80153 | | | | |

In the presence of glucose

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 8.09947 | 0.74407 | -0.19947 | H | 7.11306 | -2.33340 | -0.74931 |
| C | 7.99553 | -0.59510 | -0.93501 | H | 10.28945 | 0.59916 | -1.65941 |
| C | 9.47893 | -1.02349 | -0.93562 | H | 8.55339 | -1.85051 | 1.22700 |
| H | 7.59004 | -0.46412 | -1.94981 | C | 6.35158 | 0.65410 | 1.77932 |
| O | 7.23728 | -1.54934 | -0.19453 | O | 5.79276 | 1.40166 | -0.34869 |
| C | 9.86101 | -0.65219 | 0.51189 | H | 7.21519 | 2.36822 | 0.82023 |
| O | 10.25369 | -0.33959 | -1.89584 | H | 6.40580 | -0.44683 | 1.68351 |
| H | 9.59834 | -2.10039 | -1.12681 | O | 5.02982 | 1.11470 | 1.85758 |
| O | 9.20455 | 0.59212 | 0.72195 | H | 6.92879 | 0.93936 | 2.67896 |
| C | 6.89091 | 1.34347 | 0.51458 | N | -6.96082 | 0.03923 | -0.03340 |
| H | 8.39454 | 1.47943 | -0.97323 | C | -7.50192 | 1.33035 | -0.23539 |
| H | 10.94468 | -0.49350 | 0.63012 | C | -8.50527 | 1.82504 | 0.61697 |
| O | 9.47635 | -1.61616 | 1.44282 | C | -9.04271 | 3.09593 | 0.40937 |

| | | | | | | | |
|---|----------|----------|----------|---|-----------|----------|----------|
| C | -8.57970 | 3.90257 | -0.63621 | C | -3.71465 | -1.54224 | -0.94202 |
| C | -7.57376 | 3.41691 | -1.47896 | C | -5.08475 | -1.32764 | -0.82228 |
| C | -7.04259 | 2.14025 | -1.28913 | H | -8.86121 | 1.20721 | 1.44351 |
| C | -7.80826 | -1.03788 | 0.31606 | H | -9.82221 | 3.46441 | 1.08188 |
| C | -9.07121 | -1.17852 | -0.28677 | H | -8.99811 | 4.90001 | -0.79189 |
| C | -9.90633 | -2.23978 | 0.06508 | H | -7.20508 | 4.03302 | -2.30364 |
| C | -9.49390 | -3.18814 | 1.00765 | H | -6.26705 | 1.76293 | -1.95836 |
| C | -8.23418 | -3.05540 | 1.60259 | H | -9.39403 | -0.45098 | -1.03370 |
| C | -7.39973 | -1.98782 | 1.26939 | H | -10.88446 | -2.33319 | -0.41482 |
| C | -5.56982 | -0.17583 | -0.18231 | H | -10.14722 | -4.02213 | 1.27550 |
| C | -4.63981 | 0.75653 | 0.31567 | H | -7.89991 | -3.78411 | 2.34614 |
| C | -3.27355 | 0.54320 | 0.17558 | H | -6.42395 | -1.88447 | 1.74751 |
| C | -2.76884 | -0.61673 | -0.45316 | H | -4.99968 | 1.65400 | 0.82262 |
| C | -1.34313 | -0.90534 | -0.60825 | H | -2.58342 | 1.28505 | 0.58352 |
| C | -0.30522 | -0.11463 | -0.24898 | H | -1.12889 | -1.87695 | -1.06614 |
| C | 1.12165 | -0.42204 | -0.38207 | H | -0.51708 | 0.86498 | 0.19455 |
| C | 2.07125 | 0.54368 | 0.01577 | H | 1.70610 | 1.50184 | 0.40020 |
| C | 3.45961 | 0.34155 | -0.06162 | H | 4.95373 | -1.10430 | -0.63785 |
| C | 3.88310 | -0.90094 | -0.56881 | H | 4.45376 | 3.36178 | 0.98418 |
| B | 4.53182 | 1.44932 | 0.48178 | H | 3.32818 | -2.84029 | -1.36326 |
| O | 3.89182 | 2.75660 | 0.48350 | H | 0.89521 | -2.42903 | -1.20175 |
| C | 2.96737 | -1.88223 | -0.97385 | H | -3.35895 | -2.44824 | -1.44109 |
| C | 1.59613 | -1.65248 | -0.88527 | H | -5.78877 | -2.05954 | -1.22292 |

Table S4. Cartesian Coordinates of the DFT computed geometry for 3c

In absence of Glucose

| | | | | | | | |
|---|-----------|----------|----------|---|-----------|----------|----------|
| N | -7.61012 | 0.10266 | -0.08981 | C | -7.91507 | -2.31658 | -0.22823 |
| C | -8.28821 | -1.02471 | -0.60745 | C | -8.35106 | 1.24385 | 0.30047 |
| C | -9.34930 | -0.85884 | -1.50150 | C | -9.55033 | 1.10307 | 1.00222 |
| C | -10.02653 | -1.96392 | -1.99633 | C | -10.27677 | 2.22427 | 1.37801 |
| C | -9.64881 | -3.24970 | -1.62362 | C | -9.81342 | 3.50014 | 1.07500 |
| C | -8.58665 | -3.41717 | -0.74138 | C | -8.61610 | 3.64223 | 0.38101 |

| | | | | | | | |
|---|-----------|----------|----------|---|-----------|----------|----------|
| C | -7.89196 | 2.52561 | -0.01159 | H | -11.20387 | 2.09882 | 1.92305 |
| C | -6.21216 | 0.07729 | 0.08370 | H | -10.37842 | 4.37283 | 1.37498 |
| C | -5.38399 | -0.54799 | -0.85823 | H | -8.24805 | 4.62933 | 0.13115 |
| C | -4.01395 | -0.57455 | -0.68834 | H | -6.96521 | 2.63799 | -0.55786 |
| C | -3.40077 | 0.03096 | 0.42015 | H | -5.82869 | -1.01118 | -1.72849 |
| C | -1.96260 | 0.03947 | 0.64677 | H | -3.40689 | -1.05855 | -1.44190 |
| C | -1.02618 | -0.59067 | -0.08067 | H | -1.65367 | 0.60869 | 1.51771 |
| C | 0.41554 | -0.54731 | 0.16294 | H | -1.34322 | -1.21679 | -0.90283 |
| C | 1.28169 | -1.49838 | -0.43068 | H | 3.32907 | -2.13952 | -0.59866 |
| C | 2.65635 | -1.40325 | -0.17135 | H | 2.73267 | 1.31342 | 1.83543 |
| C | 3.18958 | -0.41923 | 0.64693 | H | 0.33430 | 1.22543 | 1.38000 |
| C | 2.33564 | 0.52285 | 1.21081 | H | -3.80278 | 1.13424 | 2.21770 |
| C | 0.97606 | 0.46129 | 0.96272 | H | -6.23765 | 1.16809 | 1.93295 |
| C | -4.24171 | 0.66212 | 1.34655 | H | 4.25455 | -0.38080 | 0.83614 |
| C | -5.61699 | 0.68139 | 1.19335 | B | 0.81593 | -2.68378 | -1.34761 |
| H | -9.64031 | 0.13924 | -1.79937 | O | -0.34934 | -3.35614 | -1.11098 |
| H | -10.84666 | -1.81829 | -2.68808 | H | -0.48848 | -4.06906 | -1.74581 |
| H | -10.17508 | -4.10984 | -2.01586 | O | 1.58045 | -3.12198 | -2.40341 |
| H | -8.28633 | -4.41179 | -0.43676 | H | 2.35443 | -2.57703 | -2.57167 |
| H | -7.09765 | -2.45091 | 0.46691 | | | | |
| H | -9.90877 | 0.11231 | 1.24636 | | | | |

In the presence of glucose

| | | | | | | | |
|---|---------|----------|----------|---|---------|----------|----------|
| C | 5.69081 | 1.68941 | 0.25107 | C | 4.47584 | 1.54906 | -0.69179 |
| C | 6.52337 | 0.40619 | 0.46898 | H | 6.35977 | 2.47184 | -0.14671 |
| C | 7.02497 | 0.61461 | 1.90593 | H | 5.93888 | 1.73585 | 3.47795 |
| H | 7.36180 | 0.34242 | -0.24627 | O | 4.81365 | 0.17866 | 2.84065 |
| O | 5.72812 | -0.76747 | 0.44893 | H | 5.20499 | -0.67522 | -0.38882 |
| C | 5.74585 | 1.17280 | 2.55170 | H | 7.76851 | 2.40870 | 1.76304 |
| O | 8.10113 | 1.52467 | 1.97992 | H | 4.82824 | -0.43513 | 2.07614 |
| H | 7.34921 | -0.33005 | 2.36539 | C | 3.11671 | 1.31370 | -0.01747 |
| O | 5.28607 | 2.10941 | 1.57703 | O | 4.60849 | 0.43594 | -1.55594 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| H | 4.40083 | 2.47881 | -1.29308 | C | 3.31812 | -4.51755 | -1.74615 |
| H | 3.22844 | 0.63077 | 0.84659 | C | 2.13696 | -3.86102 | -1.41339 |
| O | 2.34189 | 0.75280 | -1.04135 | C | -2.87092 | -2.27725 | -0.43983 |
| H | 2.66524 | 2.24869 | 0.35714 | C | -4.05709 | -1.61321 | -0.13407 |
| N | -5.26454 | 0.46581 | 0.35870 | H | -6.34083 | 2.69005 | 1.40255 |
| C | -5.59187 | 1.64903 | -0.34119 | H | -6.90638 | 4.76184 | 0.16599 |
| C | -6.15481 | 2.75072 | 0.32871 | H | -6.45900 | 4.92926 | -2.28857 |
| C | -6.47076 | 3.91529 | -0.37198 | H | -5.44516 | 2.98081 | -3.48459 |
| C | -6.21713 | 4.01270 | -1.74487 | H | -4.90842 | 0.89786 | -2.25123 |
| C | -5.64681 | 2.92261 | -2.41146 | H | -7.94441 | 0.49234 | 0.36311 |
| C | -5.34325 | 1.74784 | -1.72230 | H | -9.41497 | -0.36908 | 2.16035 |
| C | -6.10524 | -0.02821 | 1.37936 | H | -8.42831 | -1.41601 | 4.20679 |
| C | -7.50540 | 0.04851 | 1.25841 | H | -5.94158 | -1.57037 | 4.42431 |
| C | -8.32949 | -0.43894 | 2.27333 | H | -4.47126 | -0.67940 | 2.64004 |
| C | -7.77982 | -1.02878 | 3.41709 | H | -2.84750 | 1.56661 | 0.02881 |
| C | -6.38827 | -1.11721 | 3.53498 | H | -0.76045 | 0.39549 | -0.53843 |
| C | -5.55558 | -0.61695 | 2.53332 | H | -0.56718 | -3.41017 | -1.03217 |
| C | -4.06461 | -0.22143 | 0.03933 | H | 0.89212 | -0.68937 | -1.03195 |
| C | -2.85659 | 0.48348 | -0.11017 | H | 5.23528 | -1.79754 | -2.44496 |
| C | -1.68071 | -0.18262 | -0.43167 | H | 3.36992 | -5.60944 | -1.70621 |
| C | -1.65299 | -1.58563 | -0.60303 | H | 1.26968 | -4.45229 | -1.10804 |
| C | -0.43408 | -2.32691 | -0.93435 | H | -2.88533 | -3.36325 | -0.57063 |
| C | 0.78398 | -1.77052 | -1.12559 | H | -4.98773 | -2.17428 | -0.02569 |
| C | 2.04217 | -2.45103 | -1.45204 | H | 5.37325 | -4.26728 | -2.39213 |
| C | 3.17667 | -1.67168 | -1.81630 | B | 3.20665 | -0.03601 | -1.96723 |
| C | 4.35128 | -2.37239 | -2.15379 | O | 2.88869 | 0.27199 | -3.34557 |
| C | 4.43761 | -3.76618 | -2.12530 | H | 2.80066 | 1.23078 | -3.43329 |