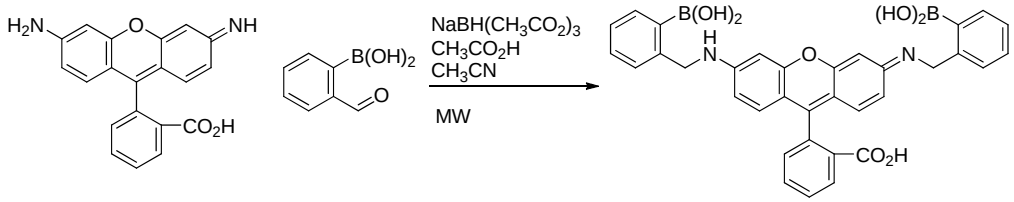
Experimental Methods and Instrumentation

All chemicals were purchased from Sigma-Aldrich and Cambridge Isotope Labs and used without further purification. Microwave synthetic procedures were performed in an Initiator™ microwave synthesizer (Biotage). NMR spectra were acquired on a Bruker AMX-400 NMR spectrometer. High-resolution mass spectrometry spectra were obtained from the Georgia State University Mass Spectrometry Facility. Absorbance spectra were collected on a Cary 50 UV-Vis spectrophotometer and Fluorescence spectra were collected on Cary Eclipse fluorescence spectrophotometer (Agilent Technologies). HPLC was carried out using a Nova Pak C18 300 Å, 4 µm, 3.9 × 150 mm (Waters, USA) column on a Waters 1525 Binary pump equipped with a Waters 2996 Photodiode Array Detector.



Synthesis of Rhodamine (bis) Boronic Acid ((E)-2-(6-((2-boronobenzyl)amino)-3-((2-boronobenzyl)imino)-3H-xanthen-9-yl)benzoic acid).

Rhodamine 110 (45 mg, 0.136 mmol), 2-formylphenyl boronic acid (100 mg, 0.667 mmol), sodium triacetoxyborohydride (90 mg, 0.425 mmol) and CH_3CN (1.7 mL) were mixed in a microwave vial (max. capacity: 2.0 mL, Biotage) containing a magnetic stir bar. Concentrated acetic acid (50 µL, 52 mg, 0.873 mmol) was then added and the vial sealed with a microwave proof cap (Biotage). The vial was stirred and irradiated while keeping the temperature at 130 ºC for 20 min. The vial then cooled to rt and the cap removed. The reaction mixture was quenched with saturated $NaHCO_3$ aqueous solution and extracted in EtOAc, dried with anhydrous Na_2SO_4 and filtered. The solvent was removed in vacuum to yield a dark red solid. Yield: 57 mg (70%). ^{1}H NMR (400 MHz, CD_3OD) δ (ppm):, 7.52-7.65 (m, 3H), 7.36-7.48 (m, 3H), 7.06-7.35 (m, 10H), 6.69 (m, 1H), 5.90 (s, 1H), 5.02 (s, 4H). ^{13}C NMR (101 MHz, CD_3OD) δ (ppm) 173.02, 155.33, 134.72, 133.31, 132.25, 131.82, 131.39, 131.25, 130.99, 130.28, 129.61, 128.88, 128.07, 125.18, 123.96, 122.19, 117.40, 72.33. HRMS ESI-FTMS *m/z* = 599.2087 $[M+H]^+$, calcd. 599.2161 for $C_{34}H_{29}B_2N_2O_7$.

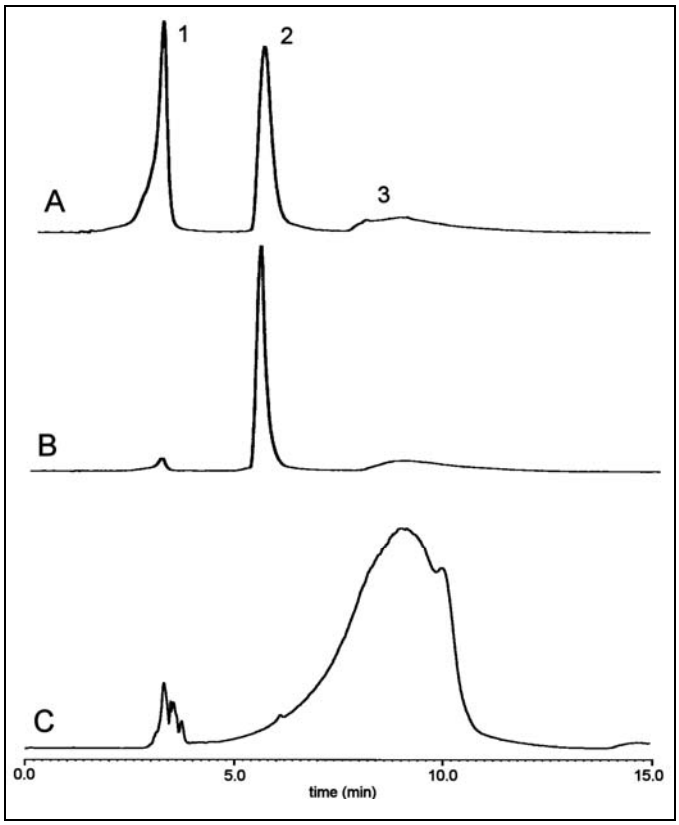


Figure S1. HPLC chromatograms from the preparation of **1** at various conditions. Peak 1 corresponds to rhodamine 110 and peak 3 to compound **1**. A) using 2 equivalents of 2-formylphenylboronic acid and irradiated to keep the reaction at 90 ºC for 8 min. B) same as above but increasing the temperature to 110 ºC and time to 10 min. C) using 5 equivalents of 2-formylphenylboronic acid and keeping the temperature at 130 ºC for 20 min. HPLC conditions: sample size: 20 µL; flow rate: 1 mL/min; mobile phase: gradient 50% MeOH/H_2O to 100% MeOH in 10 min); detection wavelength: 520 nm.

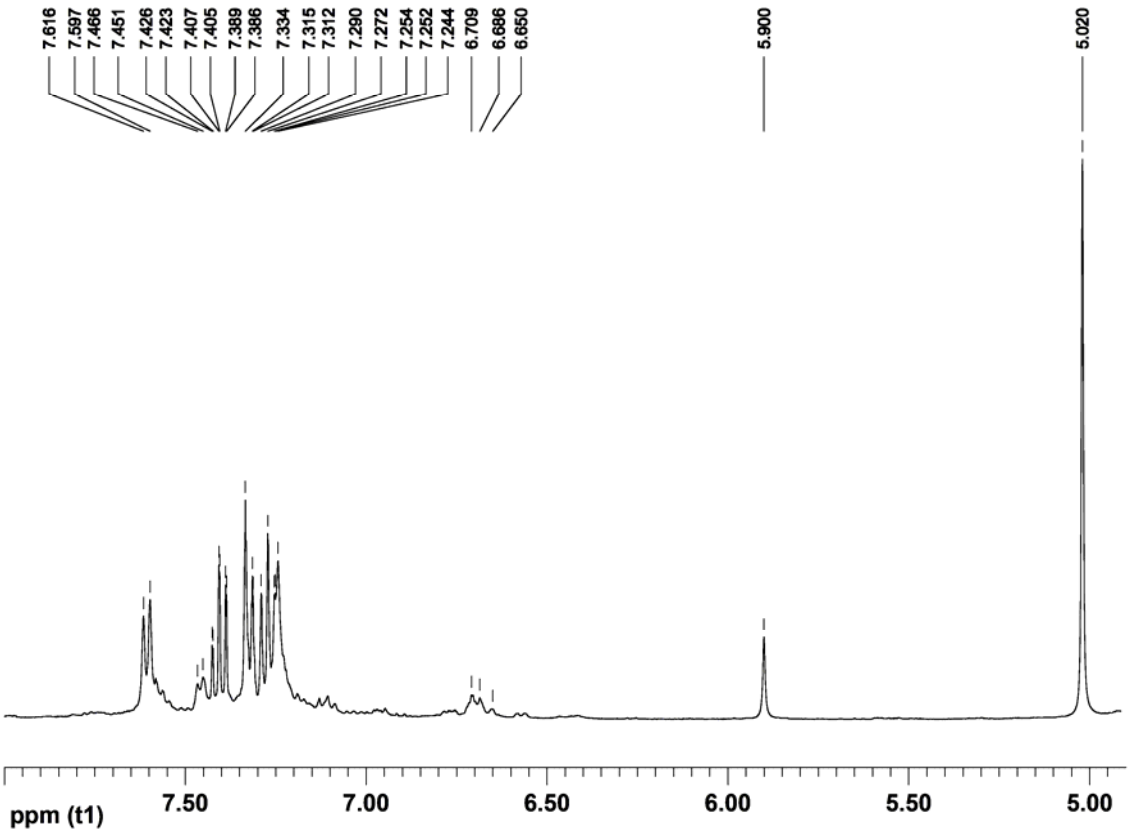


Figure S2. ^{1}H NMR of **1** in CD_3OD (400 MHz)

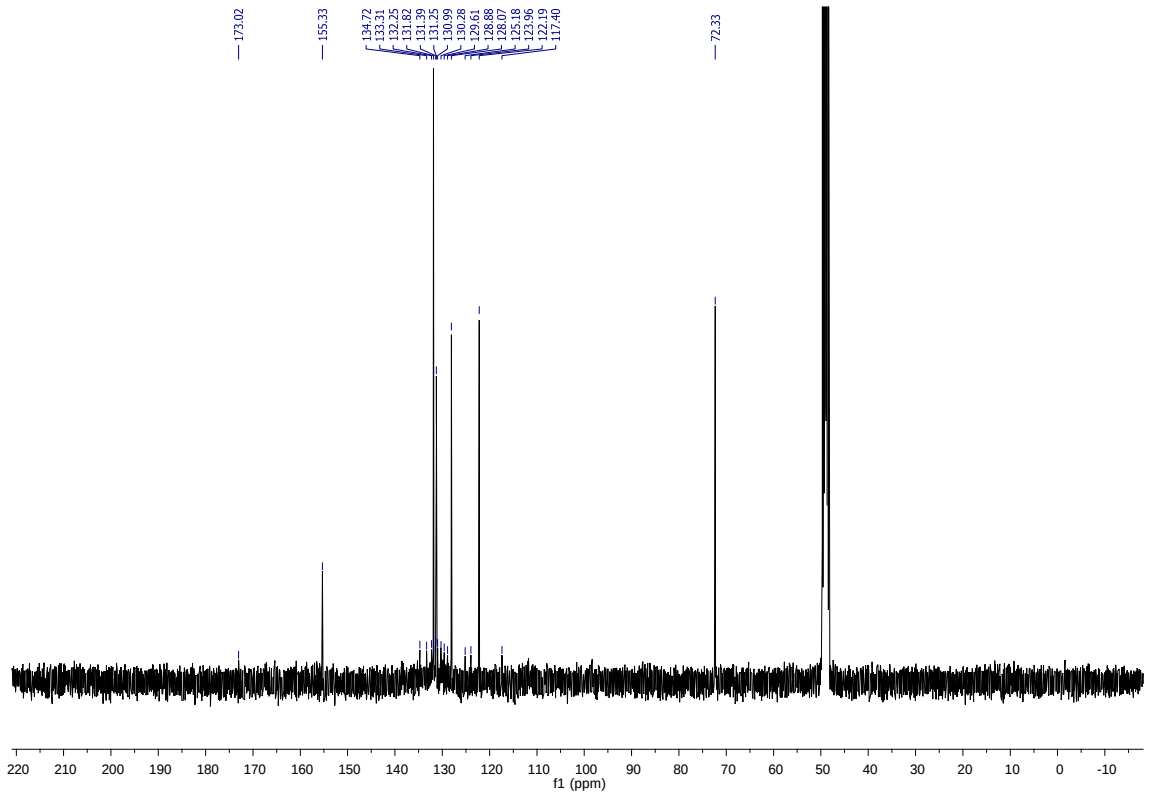


Figure S3. ^{13}C NMR of **1** (in CD_3OD 101 MHz)

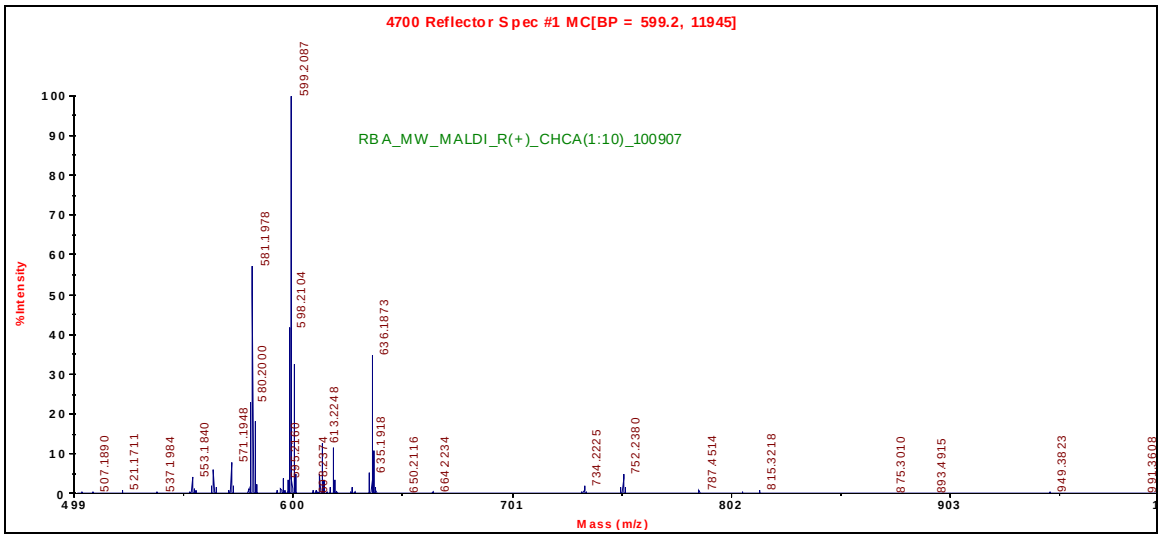


Figure S4. MALDI-TOF of **1**

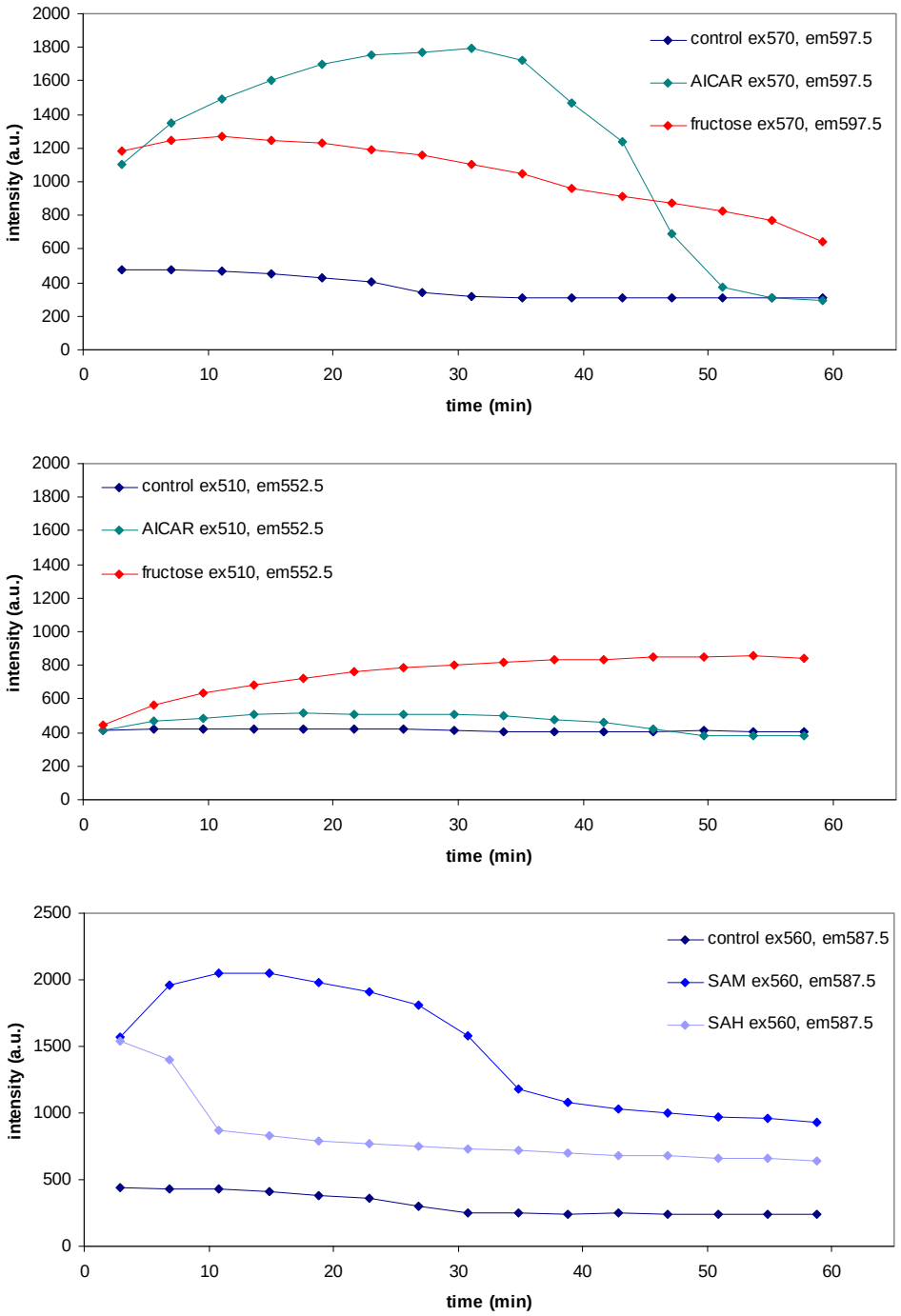


Figure S5. Intensity as a function of time. (Top) Control, AICAr and fructose emission at 597.5 nm upon excitation at 570 nm. (Center) Control, AICAr and fructose emission at 552.5 nm upon excitation at 510 nm. (Bottom) Control, SAM, and SAH emission at 587.5 nm upon excitation at 560 nm. Data correspond Figure 2 in the text.

Computational procedures.

Molecular models were built using the SYBYL™ software package version X-1.1 (Tripos Inc.) and then submitted for geometry optimization and energy minimization via MOPAC2009[1] with the following command keywords: PM6 CHARGE=-1 EF GEO-OK GNORM=0.100 MMOK SHIFT=80.

The processed file which corresponds to Figure 5 in the text is presented below in mol2 file format. To read the file, copy the text between "start of mol2 file" and "end of mol2 file" and paste it in a text editor (e.g. MS notepad) and save the file with any name with the extension ".mol2"; this file can then be opened with almost any molecular viewer program (e.g. RASMOL, UCSF Chimera, Cambridgesoft Chem3D™, SYBYL™, etc.).

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Molecular graphics images were produced using the UCSF Chimera[2] package from the Resource for Biocomputing, Visualization, and Informatics at the University of California, San Francisco (supported by NIH P41 RR001081).

References

1) MOPAC2009, James J. P. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, USA, HTTP://OpenMOPAC.net (2008).

2) UCSF Chimera--a visualization system for exploratory research and analysis. Pettersen, E. F.; Goddard, T. D.; Huang, C. C.; Couch, G. S.; Greenblatt, D. M.; Meng, E. C.; Ferrin, T. E. *J. Comput. Chem.* **2004**, *25*(13), 1605-1612.