**Supporting Information: Supramolecular Enhancement of BODIPY Singlet Oxygen Generation Using Bile Salt Micelles**

**GC-MS Chromatograms from methanol time dependence experiment**



**SI Figure 1.** (Left) Time-dependent study of DHN 🡪 juglone conversion monitored by GC-MS for reaction performed in methanol. DHN and PMB concentrations were at 4.33 x 10-4 M, 5.20 x 10-4 M. Light exposure times top to bottom were 20, 40, and 60 mins. Aqueous solutions were subject to biphasic extraction with ethyl acetate and organic layer injected into GC-MS. (Right) Signal at 4.5 mins was verified to be juglone with NIST library stored in the Agilent MS software.

GC program: Step 1: 130 ̊C for 1 min. Step 2: 20 ̊C/min heating to 300 ̊C. Step 3: maintain at 300 ̊C for 1 min.

**GC-MS Chromatograms from Sodium Cholate time dependence experiment**



**SI Figure 2.** Time-dependent study of DHN 🡪 juglone conversion monitored by GC-MS. DHN and PMB concentrations were at 4.33 x 10-4 M, 5.20 x 10-4 M, and NaCh concentration was a 11 mM respectively. Light exposure times top to bottom were 0, 15, 30, 50, and 70 mins. Aqueous solutions were subject to biphasic extraction with ethyl acetate and organic layer injected into GC-MS.

GC program: Step 1: 130 ̊C for 1 min. Step 2: 15 ̊C/min heating to 300 ̊C. Step 3: maintain at 300 ̊C for 1 min. Please note that the heating rate was slightly lowered compared to the methanol solution experiment for better resolution.

**UV-Vis spectra of Juglone**



**SI Figure 3.** UV-Vis spectrum juglone at approximately 10-5 M concentration in methanol.

**UV-Vis experiment for SOG efficiency of *b*-CD and *g*-CD**



**SI Figure 4.** Change in UV-Vis spectrum of solution of BODIPY (4.92 x 10-5 M) and DHN (5.68 x 10-5 M) in water, in presence of 3 mM host (left is *b*-CD, and right is *g*-CD) exposed to visible light under oxygen purging conditions, and recorded in 5 min duration. Time of exposure to light while purged with oxygen starts at 0 mins with 5 min increments for each run up to a maximum of 50 mins.

**Plot of relative rates of singlet oxygen generated using different media**

**SI Figure 5.** Plot showing relative rates of singlet oxygen generation as observed through the oxidation of DHN to produce juglone as the probe reaction in different media and corresponding spectral change at 258 nm for different media explored in this project.



**Coordinates of geometry-optimized sodium cholate with BODIPY (PMB) in water medium (IPCM) performed in HF STO-3G**

HEADER

REMARK Spartan'20 exported M0001

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HETATM 3 C UNK 0001 1.954 9.719 -2.728

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HETATM 5 C UNK 0001 1.142 9.004 -1.606

HETATM 6 C UNK 0001 1.156 7.471 -1.818

HETATM 7 H UNK 0001 2.193 7.200 -2.008

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HETATM 11 C UNK 0001 -1.540 6.132 -1.525

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HETATM 13 C UNK 0001 -3.643 5.410 -0.083

HETATM 14 C UNK 0001 -5.146 5.217 -0.428

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HETATM 17 C UNK 0001 -7.842 5.021 -1.817

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