Supporting Information

Development of Reversible Fluorescence Probes Based on Redox Oxoammonium Cation for Hypobromous Acid Detection in Living Cells

Fabiao Yu,[a,b] Ping Song,[a] Peng Li,[a] Bingshuai Wang,[a] and Keli Han[a]*

[a]State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences (CAS), 457 Zhongshan Road, Dalian 116023, P. R. China
E-mail: klhan@dicp.ac.cn
[b]School of Chemical Engineering, Dalian University of Technology, Dalian 116024, P. R. China;
E-mail: yufabiao@163.com

Contents:

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1. General Experimental Section

Materials: The solution of the probe *m*Cy-TemOH and Cy-TemOH (acetonitrile, 1.0 mM) could be maintained in refrigerator at 4°C. 2-[4-Chloro-7-(1-ethyl-3,3-dimethyl(indolin-2-ylidene)]-3,5-(propane-1,3-diyl)-,3,5-heptatrien-1-yl)-1-ethyl-3,3-dimethyl-3H-indolium (Cy.7.Cl) was synthesized in our laboratory.[1] The cell-permeant SYTO-16 green fluorescent nucleic acid stain (SYTO-16 dye) exhibited bright, green fluorescence upon binding to nucleic acids. The blue fluorescent Hoechst dyes are cell permeable nucleic acid stains. The fluorescence of these dyes is very sensitive to DNA conformation and chromatin state in cells. The regents were purchased from Invitrogen Corporation, and used according to the manufacturer's instructions. HOCl was standardized at pH 12 ($\varepsilon_{292\ nm}$ = 350 $M^{-1}cm^{-1}$).[2] HOBr was prepared by adding HOCl to a small excess of NaBr in water and standardizing at pH 12 ($\varepsilon_{329\ nm}$ = 332 $M^{-1}cm^{-1}$).[3] [HOBr] used in Fig.1: 0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110 μM. HOCl and HOBr can readily pass through the plasma membrane into the cell because of their electrical neutrality and small molecular size being comparable to those of water.[4] Methyl linoleate (MeLH) and 2,2'-azobis-(2,4-dimethyl)valeronitrile (AMVN) were used to produce MeLOOH.[5] *Tert*-butylhydroperoxide (*t*-BuOOH) and cumene hydroperoxide (CuOOH) could also use to induce ROS in biological systems.[6] All other chemicals were from commercial sources and of analytical reagent grade, unless indicated otherwise. RAW264.7 cells (mouse macrophages cell line) were purchased from the Committee on type Culture Collection of Chinese Academy of Sciences. Ultrapure water was used throughout.

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Instruments: Fluorescence spectra were obtained by FluoroMax-4 Spectrofluorometer with a Xenon lamp and 1.0-cm quartz cells. Absorption spectra were measured on Lambda 35 UV-visible spectrophotometer (PerkinElmer). ^{1}H and ^{13}C NMR spectra were taken on a Bruker spectrometer. The fluorescence images of cells were taken using a LTE confocal laser scanning microscope (Olympus FV1000 confocal laser-scanning microscope) with objective lens (×40).

Absorption Analysis: Absorption spectra were obtained with 1.0-cm glass cells. The probes (acetonitrile, 0.1 mL, 1.0 mM) was added to a 10.0-mL color comparison tube. After dilution to 10 μM with 0.2 M PBS buffers, then various concentrations HBrO was added. The mixture was equilibrated for 15 min before measurement.

Fluorescence Analysis: Fluorescence emission spectra were obtained with a Xenon lamp and 1.0-cm quartz cells. The probes (acetonitrile, 0.1 mL, 1.0 mM) were added to a 10.0-mL colorcomparison tube. After dilution to 10 μM with 0.2 M PBS buffers, HBrO was added. The mixture was equilibrated for 15 min before measurement.

Confocal Imaging: Fluorescent images were acquired on Olympus FV1000 confocal laser-scanning microscope with an objective lens (×40). Cell imaging was carried out after washing cells with fresh complete medium (RPMI-1640+20% FBS, 3×1 mL).

Cell Culture: Murine RAW264.7 macrophage cells (ATCC, USA) were maintained following protocols provided by the American Type Culture Collection. Cells were seeded at a density of 1×10^{6} cells mL^{-1} for confocal imaging in RPMI 1640 Medium supplemented with 20% fetal bovine serum (FBS), $NaHCO_3$ (2 g/L), and 1%antibiotics (penicillin/streptomycin, 100 U/ml). Cultures were maintained at 37 °C under a humidified atmosphere containing 5% CO_2. Cultures were maintained at 37 °C under a humidified atmosphere containing 5% CO_2. The cells were subcultured by scraping and seeding on 33 mm coverglass slides according to theinstructions from the manufacturer.

2. Synthesis and Characterization of Compounds

The syntheses of the two fluorescent molecules were performed in a straightforward way. The fluorophore Cy and 4-amino-2,2,6,6-tetramethylpiperidine-N-oxyl (TempO) were dissolved in anhydrous DMF under Ar atmosphere at 40 ^{o}C for 4h. After the removal of solvent under vacuum, the intermediates were afforded by preparative thin-layer chromatography. Interestingly, we obtained two molecules, *mero*Cyanine-TempO (*m*Cy-Tem) and Cyanine-TempO (Cy-Tem) in one pot. After reduced the two compounds by ascorbic acid, the target products, *m*Cy-TemOH and Cy-TemOH, were afforded finally.

Cy-Tem was constructed *via* an S_N1 reaction mechanism where the *meso*-chlorine atom of heptamethine dye is substituted with nucleophilic aminoalkyl (Scheme S1).[7] A proposed reaction mechanism for the synthesis of TempO derivative *m*Cy-Tem is shown in Scheme S2. Amino addition reaction of TempO moiety at the $C_{2'(6')}$ position of heptamethine polymethine chain to afford *m*Cy-Tem. The ground-state electron density of a representative heptamethine cyanine can reveal the chemical reactivity of cyanine dyes (Fig. S1).[8] the level of difficulty to electrophilic addition at the carbons is in the decreasing order of $C_{2(2")} > C_{2'(6')} > C_{4'}$. However, in the presence of TempO, the steric hindrance of $C_{2(2")}$ position accelerates the competitive addition at $C_{2'(6')\ 4'}$ positions. The solvent might also play an important role in the mechanism.[9]

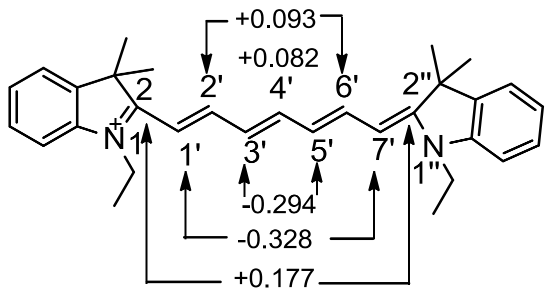
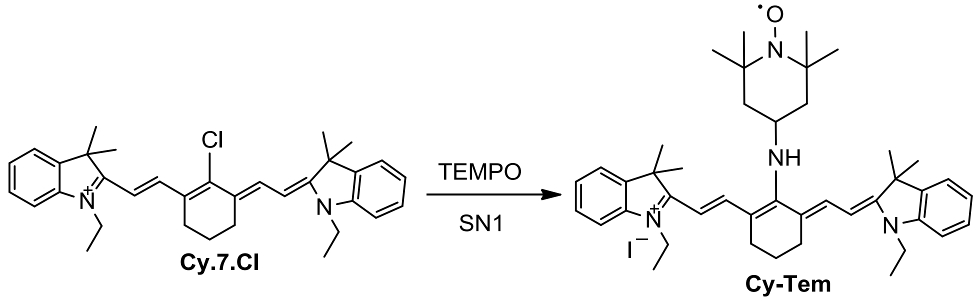
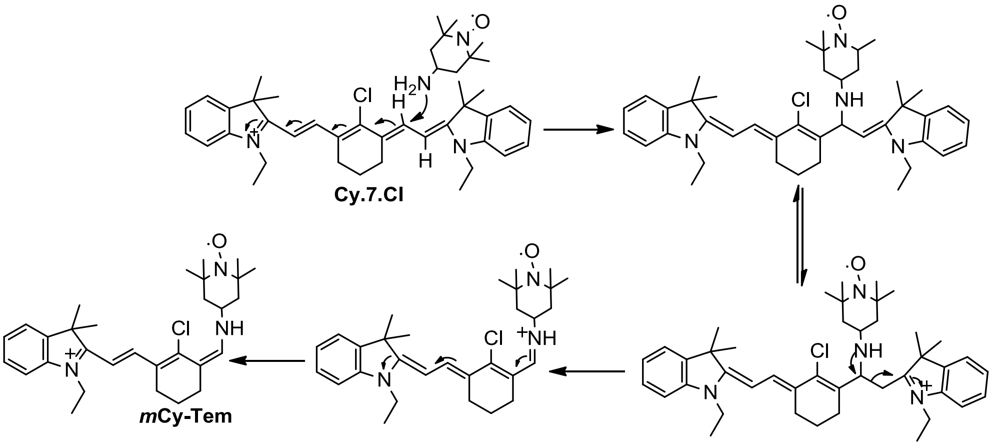


Fig. S1 Point charges at carbon atoms of heptamethine cyanine as obtained from ampac calculation method.[8]



Scheme S1. Proposed S_N1 Reaction Mechanism for Cy-Tem



Scheme S2. Proposed Amino Addition Reaction Mechanism for *m*Cy-Tem

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Synthesis of *m*Cy-Tem: Cy.7.Cl (1.0 g, 1.56 mmol), 4-amino-2,2,6,6-tetramethylpiperidine-N-oxyl (TempO) (1.0g, 5.84 mmol) were dissolved in 15 mL of anhydrous DMF in a 25-mL round bottom flask under Ar for 4 h at 40 °C.[10] Then the solvent was evaporated on a rotary evaporator until dry below 40 °C. The solid was purified on preparative thin-layer chromatography eluted with dichloromethane. 0.425 g, 0.858 mmol. Yield: 55 %. All above operations are carried out under argon atmosphere. Characterization of acid form (*m*Cy-Tem, blue powder): ^{1}HNMR (400 MHz, $CDCl_3$-D_1, 0.1% CD_3COOD-D_4) δ(ppm): 8.00 (s, 1H), 7.30-7.15 (m, 4H), 6.50 (s, 1H), 5.84 (s, 1H), 5.28 (s, 1H), 4.02 (m, 2H), 2.96 (s, 2H), 2.88 (s, 2H), 2.79 (s, 1H), 1.87-1.58 (m, 15H), 1.40-1.08(m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$-D_1) δ(ppm):168.8, 162.6, 142.4, 140.7, 140.1, 128.5, 127.7, 123.8, 122.2, 122.0, 121.5, 120.0, 109.2, 105.54, 96.3, 59.2, 54.6, 45.5, 39.3, 32.9, 29.6, 29.3, 28.6, 25.1, 24.4, 22.7, 22.0, 20.1, 12.1, 11.0p . LC-MS (API-ES): *m/z* $C_{30}H_{42}ClN_3O^+$ Calcd 495.3011, found 495.3515. Elemental Analysis: Calcd C, 72.63; H, 8.53; N, 8.47, found C, 72.62; H, 8.52; N, 8.47. Characterization of alkaline form (*m*CyOH-Tem, brown powder): ^{1}HNMR (400 MHz, $CDCl_3$-D_1) δ(ppm): 8.62 (s, 1H), 8.31 (s, 1H), 7.51-7.03 (m, 3H), 6.57-6.56 (d, 2H), 6.12(s, 1H), 5.41-5.38 (d, 1H), 3.62-3.54 (m, 2H), 2.53 (m, 4H), 2.17-1.42 (m, 16H), 1.31-1.10 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$-D_1) δ(ppm):170.4, 166.5, 163.0, 157.9, 139.8, 137.8, 136.8, 135.5, 124.2, 123.2, 120.8, 118.9, 118.1, 117.4, 117.0, 114.6, 104.6, 101.1, 94.3, 89.6, 43.7, 43.2, 34.5, 27.3, 25.2, 24.7, 22.6, 21.8, 18.3, 11.0. LC-MS (API-ES): *m/z* $C_{30}H_{43}ClN_3O_2$ Calcd 512.3044, found $[M\text{-}H]^+$ 511.3406. Elemental Analysis: Calcd C, 70.22; H, 8.45 N, 8.19, found C, 70.21; H, 8.44 N, 8.19.

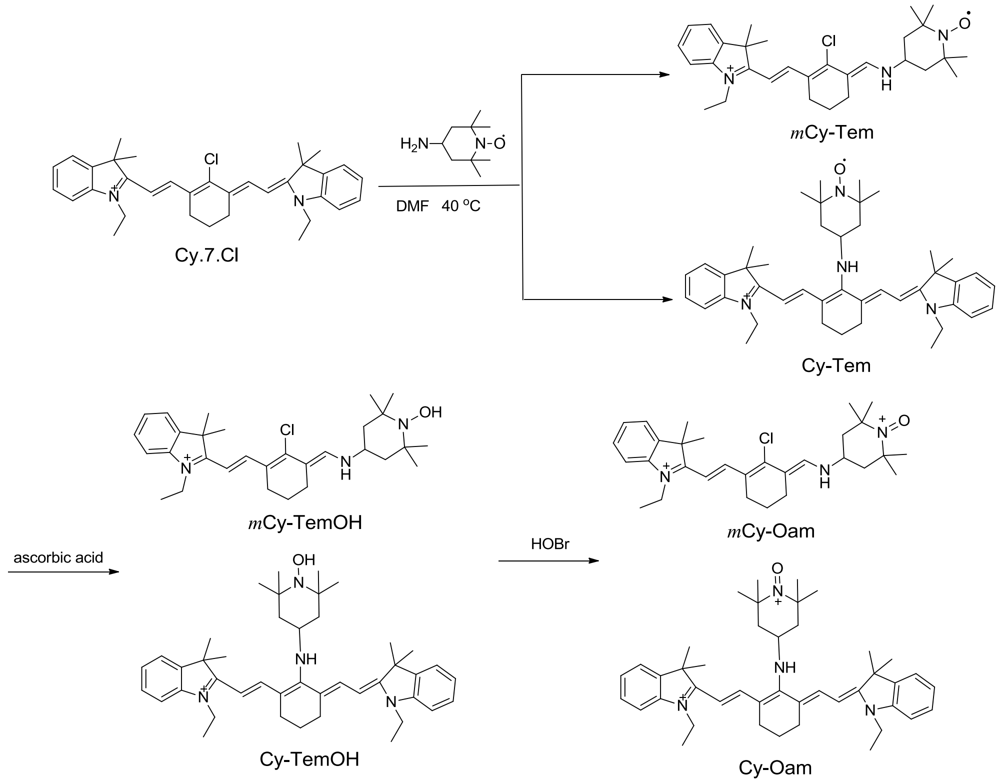
Characterization of *m*Cy-TemOH: *m*Cy-Tem (0. 1 g) was dissolved in 5 mL acetonitrile. Subsequently, 10 equiv. of ascorbic acid was added. The mixture was equilibrated for 15 min.[11] The solvent was evaporated on a rotary evaporator until dry. The solid was purified on preparative thin-layer chromatography eluted with ethyl acetate. LC-MS (API-ES): *m/z* $C_{30}H_{43}ClN_3O^+$ Calcd 496.3089, found [M^+] 496.3060. Elemental Analysis: Calcd C, 72.48; H, 8.72; N, 8.45, found C, 72.48; H, 8.73; N, 8.46.

Characterization of *m*Cy-Oam: *m*Cy-TemOH (0. 1 g) was dissolved in a mixture of 3 mL CH_2Cl_2 and 3 mL water. Subsequently, 100 equiv. of HOBr was added. The mixture was equilibrated for 15 min.[12] Then the mixture was extracted by ethyl acetate. Then washed the organic phase 3 times by KBr (10 %) solution (3×5 mL). The solvent was evaporated on a rotary evaporator until dry. The solid was purified on preparative thin-layer chromatography eluted with ethyl acetate. LC-MS (API-ES): *m/z* $C_{30}H_{42}ClN_3O^{2+}$ Calcd 495.3005, found [M^{2+}] 247.6500. Elemental Analysis: Calcd C, 54.93; H, 6.45; N, 6.41, found C, 54.92; H, 6.45; N, 6.42.

Synthesis of Cy-Tem: Cy.7.Cl (1.0 g, 1.56 mmol), 4-amino-2,2,6,6-tetramethylpiperidine-N-oxyl (TempO) (1.0g, 5.84 mmol) were dissolved in 15 mL of anhydrous DMF in a 25-mL round bottom flask under Ar for 4 h at 40 ^{o}C.[10] Then the solvent was evaporated on a rotary evaporator until dry below 40 ^{o}C. The solid was purified on preparative thin-layer chromatography eluted with ethyl acetate affording green powder. 0.353 g, 0.546 mmol. Yield: 35 %. All above operations are carried out under argon atmosphere. ^{1}HNMR (400 MHz, CD_3OD-D_4) δ(ppm): 8.63 (s, 1H), 7.54-7.06 (m, 5H), 6.98-6.56 (m, 3H), 5.45-5.44 (d, 2H), 4.11 (s, 1H), 3.65-3.50 (q, 4H), 2.89(t, 4H), 2.51 (t, 4H), 1.93-1.29 (m, 22H), 1.19-1.03 (m, 12H). ^{13}C NMR (100 MHz, CD_3OD-D_4) δ(ppm): 161.8, 161.4, 160.4, 145.6, 145.1, 143.2, 142.5, 141.8, 141.4, 140.2, 130.8, 129.9, 129.8, 129.6, 128.9, 128.8, 128.7, 126.6, 126.0, 124.6, 123.9, 123.6, 123.5, 122.7, 121.3, 112.1, 111.6, 109.8, 107.5, 99.9, 93.2, 62.8, 59.7, 47.8, 47.0, 40.2, 37.8, 36.5, 35.6, 33.0, 32.9, 32.8, 30.7, 30.5, 30.4, 30.2, 28.7, 28.6, 28.33, 28.0, 27.9, 27.5, 26.8, 25.4, 24.5, 23.6, 22.7, 20.7, 20.5, 14.4, 12.9, 12.6, 12.4, 11.3. LC-MS (API-ES): *m/z* $C_{43}H_{58}N_4O^+$ Calcd 646.4605, found 646.5214. Elemental Analysis: Calcd C, 79.83; H, 9.04; N, 8.66, found C, 79.84; H, 9.04; N, 8.66.

Characterization of Cy-TemOH: Cy-Tem (0.1 g) was dissolved in 5 mL acetonitrile. Subsequently, 10 equiv. of ascorbic acid was added. The mixture was equilibrated for 15 min.[11] The solvent was evaporated on a rotary evaporator until dry. The solid was purified on preparative thin-layer chromatography eluted with ethyl acetate. LC-MS (API-ES): *m/z* $C_{43}H_{59}N_4O^+$ Calcd 647.4683, found [M^+] 647.4603. Elemental Analysis: Calcd C, 79.71; H, 9.18; N, 8.65, found C, 79.70; H, 9.19; N, 8.65.

Characterization of Cy-Oam: Cy-TemOH (0.1 g) was dissolved in a mixture of 3 mL CH_2Cl_2 and 3 mL water. Subsequently, 100 equiv. of HOBr was added. The mixture was equilibrated for 15 min.[12] Then the mixture was extracted by ethyl acetate. Then washed the organic phase 3 times by KBr (10 %) solution (3×5 mL). The solvent was evaporated on a rotary evaporator until dry. The solid was purified on preparative thin-layer chromatography eluted with ethyl acetate. LC-MS (API-ES): *m*/*z* $C_{43}H_{58}N_4O^{2+}$ Calcd 646.4600, found [M^{2+}] 343.3444. Elemental Analysis: Calcd C, 64.02; H, 7.25; N, 6.94, found C, 64.03; H, 7.24; N, 6.94.



Scheme S3. Synthesis of the Probe *m*Cy-TemOH and Cy-TemOH

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3. Photostability of the Compounds mCy-TemOH and Cy-TemOH

The photostability of the probes was tested by measuring the fluorescent response during 1 h. Fig. S2 shows the time courses of fluorescence intensity of the probes (10 μM) in 0.2 M PBS buffer solution with pH 7.40 at room temperature. The fluorescence intensities were measured at $\lambda_{ex/em}$ =

610/632 nm for mCy-TemOH, $\lambda_{ex/em}$ = 702/755 nm for Cy-TemOH. The experiments indicate that the probes are stable to the medium, light, and air.

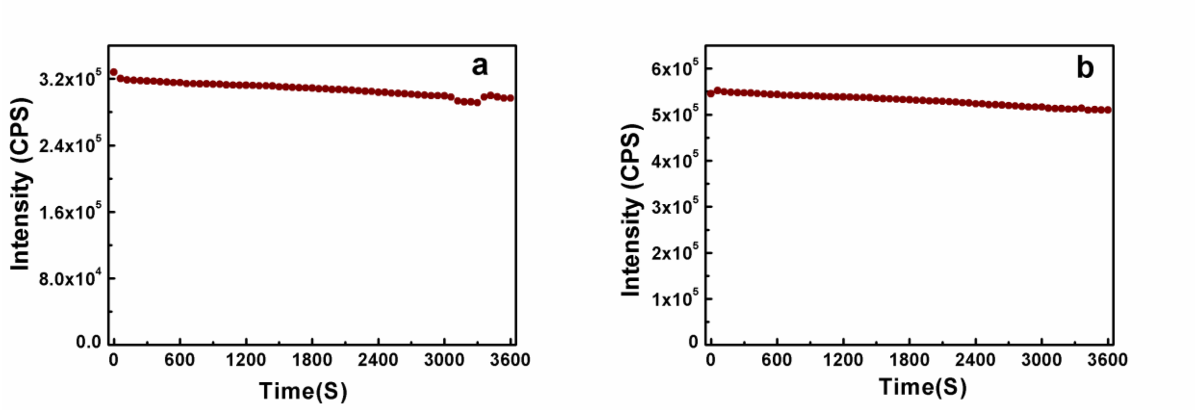
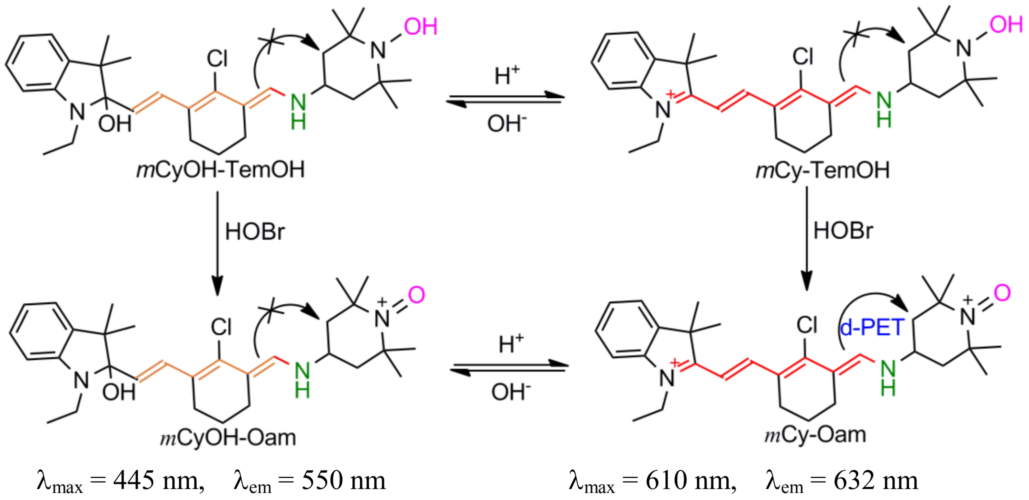


Fig. S2 Time courses of mCy-TemOH and Cy-TemOH were measured by spectrofluorometer $\lambda_{ex/em}$ = 610/632 nm and $\lambda_{ex/em}$ = 702/755 nm, respectively. The concentrations of probes were 10 μM in 0.2 M PBS buffer pH 7.40 respectively. a) For mCy-TemOH. b) For Cy-TemOH.

4. Effect of pH Values

We evaluated the effects of pH on the spectral properties of the two probes in 0.2 M PBS buffer. Fluorescence pH titrations were performed in buffer solution at a probe concentration of 10 μM in 0.2 M PBS respectively. It is interesting that *m*Cy-TemOH undergoes distinct color change from yellow to blue (Fig. S3a). Fig. S3 shows the pH dependence on the absorption spectrum of *m*Cy-TemOH. *m*Cy-TemOH exhibits absorption maxima at 445 nm and 610 nm at neutral pH values. Upon increasing pH, λ_{max} = 610 nm band keeps decreasing its intensity, and λ_{max} = 445 nm band increasing, resulting in big changes in the absorption spectrum and corresponding the fluorescence spectrum. Spectral changes of such kind can be attributed to the addition of a hydroxyl ion to an electrophilic site of the dye structure (Scheme S4, *m*CyOH-TemOH). This reaction interrupts the conjugation system and gives a hypsochromic shift.[13] The proposed acide-base equilibrium is shown in Scheme S4. The λ_{max} = 445 nm band can be related to *m*CyOH-TemOH (alkaline form), the proposed mechanism for the interaction of the hydroxyl anion with the dye molecule and the subsequent perturbation of the π system. When fixed pH value at 7.4, *m*CyOH-TemOH shows absorption maxima at 445 nm and fluorescence maxima at 550 nm. Reaction of *m*CyOH-TemOH with HOBr triggered chemoselective oxidation of TemOH to oxoamonium cation. The fluorescence intensity at 550 nm does not change. *m*Cy-TemOH exhibits absorption maxima at 610 nm and fluorescence maxima at 632 nm. The fluorescence intensity at 632 nm becomes lower after added HOBr. According to a literature method,[14] affording a p*K*a value of ~7.5. As is shown in Fig. S4, Cy-TemOH has hardly effect on fluorescence intensity by the pH of the mediums within the range from 4.0 to 10.0. These results imply that the probe will work well under physiological conditions (pH=7.4).



Scheme S4. The proposed acide-base equilibrium for *m*Cy-TemOH and *m*CyOH-TemOH

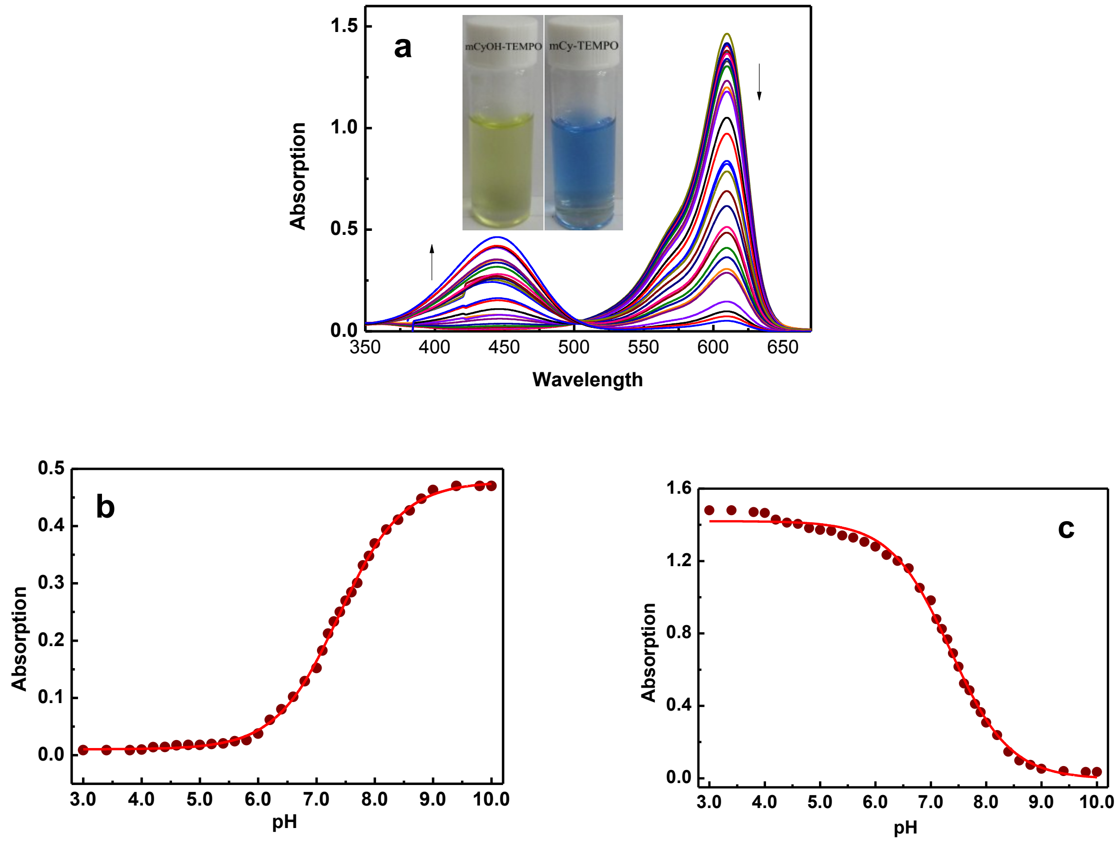


Fig. S3 (a) Dependence on pH of the absorption in 0.2 M buffered aqueous solution (PBS) 10 μM *m*Cy-TemOH. From acidic to basic conditions: pH 3.0, 3.4, 3.8, 4.0, 4.2, 4.4, 4.6, 4.8, 5.0, 5.2, 5.4, 5.6, 5.8, 6.0, 6.2, 6.4, 6.6, 6.8, 7.0, 7.2, 7.4, 7.6, 7.80, 8.0, 8.2, 8.4, 8.6, 8.8, 9.0, 9.4, 9.8, 10.0; b) and c) Nonlinear fitting of the pH-dependent extinction coefficient $\varepsilon_{445\ nm}$ and $\varepsilon_{610\ nm}$, respectively.

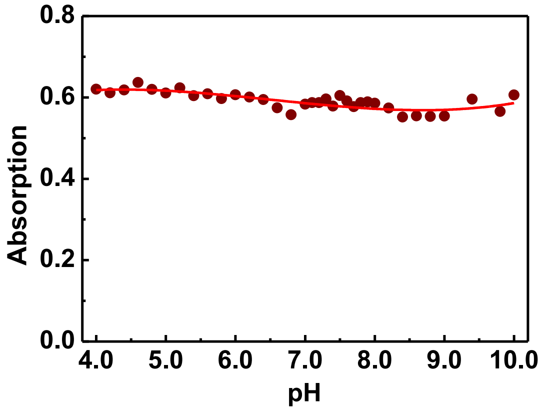


Figure S4. Nonlinear fitting of the pH-independent extinction coefficient $\varepsilon_{702\ nm}$ of Cy-TemOH (10 μM). The absorption in 0.2 M buffered aqueous solution (PBS), From acidic to basic conditions: pH 4.0, 4.2, 4.4, 4.6, 4.8, 5.0, 5.2, 5.4, 5.6, 5.8, 6.0, 6.2, 6.4, 6.6, 6.8, 7.0, 7.2, 7.4, 7.6, 7.80, 8.0, 8.2, 8.4, 8.6, 8.8, 9.0, 9.4, 9.8, 10.0.

[13] (a) Lipowska M., Patterson S. E., Patonay G., Strekowski L., Journal of Heterocyclic Chemistry 1993, 30, 1177. (b) C. Encinas, S. Miltsov, E. Otazo, L. Rivera, M. Puyol, J. Alonso, Dyes and Pigments, 2006, 71, 28.
[14] B. Tang, F. Yu, P. Li, L. Tong, X. Duan, T. Xie, X. Wang, *J. Am. Chem. Soc.*, **2009**, 131, 3016.

5. Coexist Various Biologically Relevant Analytes Interference Test

Next, we examined the reactivity of mCy-TemOH and Cy-TemOH toward various reactive oxygen species (ROS) respectively. The responses of the two probes were found to be selective for HOBr over other ROS. Upon addition of HOBr in phosphate buffered solution (0.2 M PBS pH 7.4), both of the probes showed large fluorescence decrease within 15 min (Fig. S5). HOCl and H_2O_2 induced limited fluorescence responses. However, the intensity of the fluorescence decrease was far weaker than that caused by HOBr. To confirm the chemoselective hydroxylamine switch could turn on only upon incubation with HOBr, the time courses of *m*Cy-TemOH and Cy-TemOH with various ROS for 30 min were tested. As demonstrated in Fig. S5, the two probes can selectively respond to HOBr within 15 min regardless of other relevant species. Summarizing the experimental results, it is clearly demonstrated that the selective oxidation of hydroxylamine to Oam can be used for fluorescence detection of HOBr under simulated physiological conditions.

Since Oam could be reduced by ascorbic acid, we studied the reversibility of the reaction between oxidized probes and ascorbic acid. Considering the complex and diverse anti-oxidizing environment in cells, an additional important work of the probe was carried out to determine which the antioxidant could trigger the fluorescent d-PET switch off efficaciously. As indicated in Fig. S6 and Fig. S7, the probe displayed the excellent selectivity response to ascorbic acid. The oxidized probes were reduced upon addition of ascorbic acid and showed strong fluorescence.

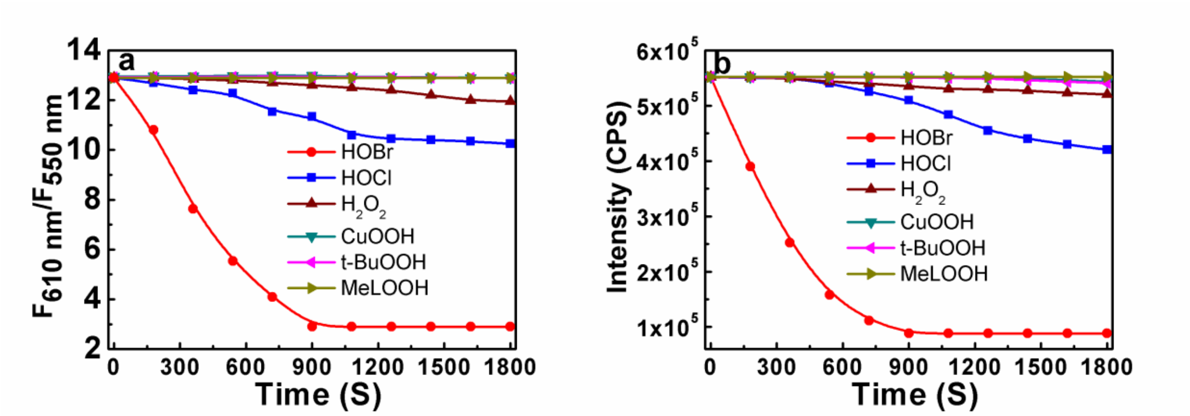


Fig. S5 Fluorescence responses and time courses of 10 μM probes to biologically relevant reactive oxygen species for 30 min. Data were obtained in 0.2 M PBS buffer pH 7.4 at 25°C. a) Ratiometric fluorescence responses ($F_{610\ nm}/F_{550\ nm}$, λ_{ex} = 445 nm 610 nm respectively) of *m*Cy-TemOH to various ROS. b) Fluorescence responses of Cy-TemOH at 750 nm (λ_{ex} = 710 nm) to various ROS. Species shown: HOBr, HOCl, H_2O_2, cumene hydroperoxide (CuOOH), tert-butyl hydroperoxide (t-BuOOH), and methyl linoleate hydroperoxide (MeLOOH) all at 100 μM.

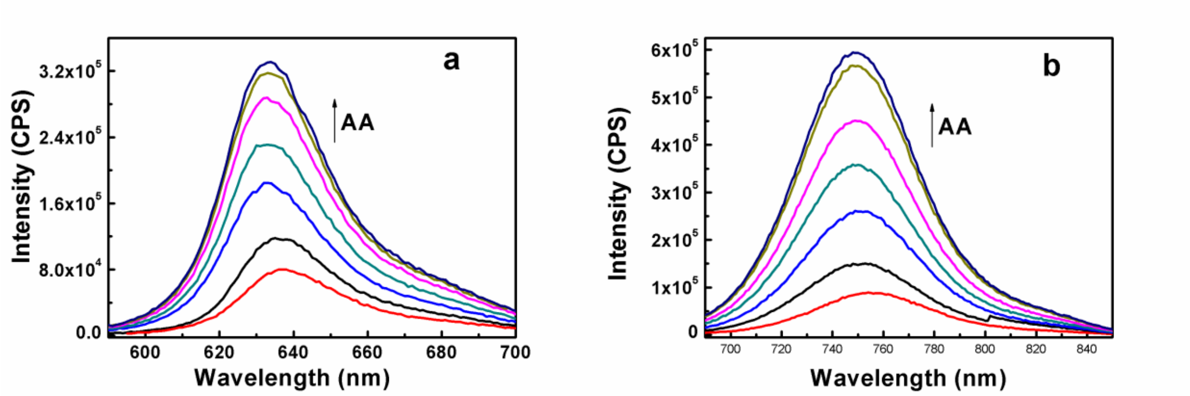


Fig. S6 Time-dependent fluorescence responses of 10 μM probes to ascorbic acid (AA). Spectra were acquired in 0.2 M PBS, pH 7.4 at 25°C after incubation of the probes with 100 μM ascorbic acid for 0, 3, 6, 9, 15 and 18 min. a) For mCy-TemOH, $\lambda_{ex/em}$ = 610/632 nm. b) For Cy-TemOH, $\lambda_{ex/em}$ = 702/755 nm.

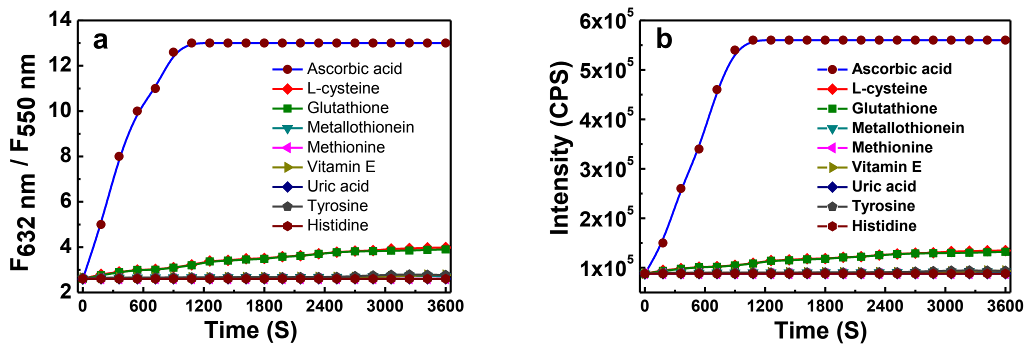


Fig. S7 Time courses of the responses of *m*Cy-Oam and Cy-Oam to various reducing materials. 10 μM probes were treated with various reducing materials for 60 min: ascorbic acid, L-cysteine, glutathione, metallothionein, methionine, vitamin E, uric acid, tyrosine, and histidine all at 100 μM. Data were obtained in 0.2 M HEPES buffer pH 7.4 at 25°C. a) For *m*Cy-Oam. b) For Cy-Oam.

6. MTT Assay

3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay: RAW264.7 cells (10^6 cell mL^{-1}) were dispersed within replicate 96-well microtiter plates to a total volume of 200 μL $well^{-1}$. Plates were maintained at 37 °C in a 5% CO_2/95% air incubator for 4h. RAW264.7 cells were then incubated for 24h upon different concentrations probe of 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7} and 10^{-8} M respectively. MTT solution (5.0 mg/mL, PBS) was then added to each well. After 4h, the remaining MTT solution was removed, and 200 μL of DMSO was added to each well to dissolve the formazan crystals. Absorbance was measured at 570 nm in a TRITURUS microplate reader. Calculation of IC50 values was done according to Huber and Koella.[15]

To evaluate cytotoxicity of the probe, we performed an MTT assay in RAW264.7 cells with probe concentrations from 0.01 μM to 10.0 mM. The result showed IC50 = 101 μM for mCy-TemOH, IC50 = 200 μM for Cy-TemOH, which clearly demonstrated that the probe was of low toxicity to cultured cell lines under the experimental conditions at the concentration of 10 μM.

[15] W. Huber, J. C. Koella, *Acta Trop.* **1993**, *55*, 257–261.

7. Additional Fluorescent Confocal Microscopy Images for Fig. 3 and Fig. 4

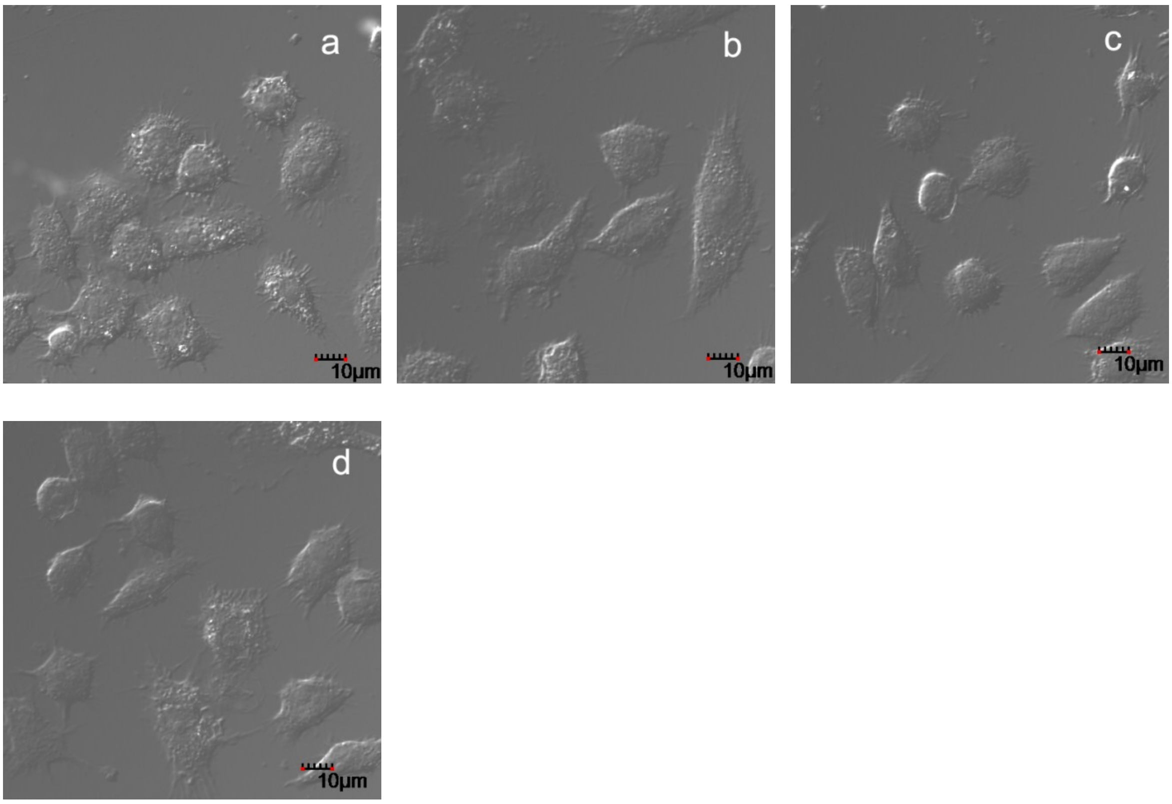


Fig. S8 Brightfield images of cells in Fig. 3. (a) Brightfield images of Fig. 3a. (b) Brightfield images of Fig. 3b. (c) Brightfield images of Fig. 3c. (d) Brightfield images of Fig. 3d.

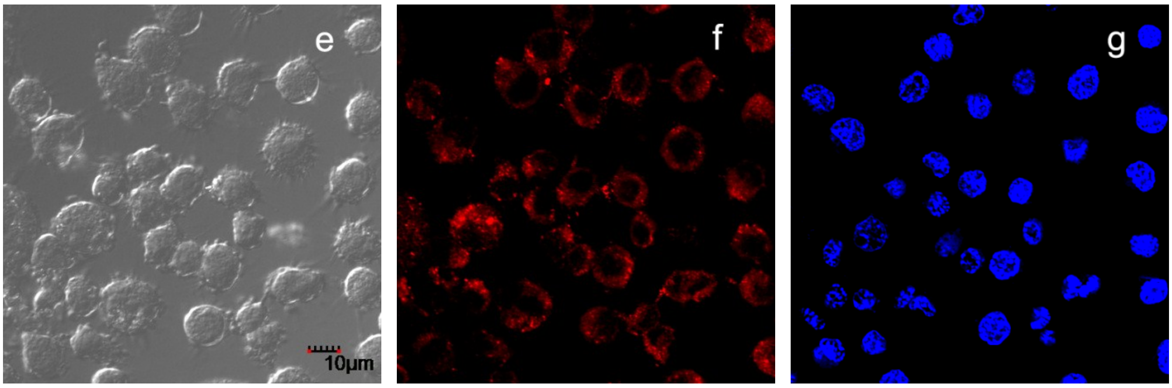


Fig. S9 (e) Brightfield images of Fig. 3e. (f) Red channel of Fig. 3e. (g) Blue channel of Fig. 3e.

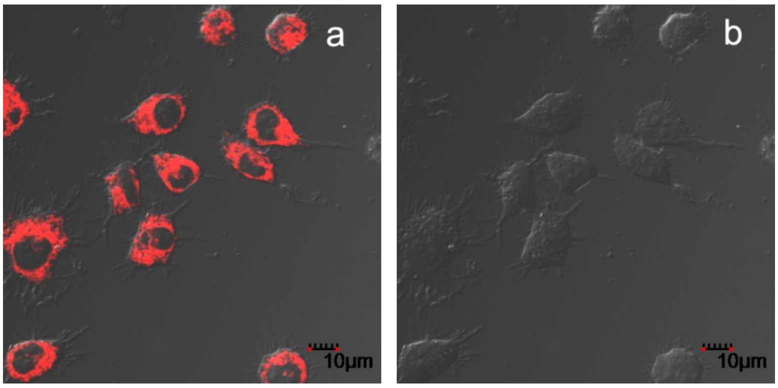


Fig. S10 (a) Merged images of brightfield (b) and red channel (Fig. 4a). (b) Brightfield images of Fig. 4a.

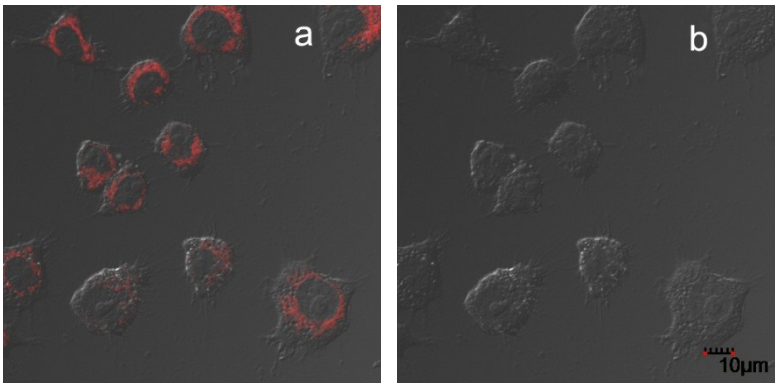


Fig. S11 (a) Merged images of brightfield (b) and red channel (Fig. 4b). (b) Brightfield images of Fig. 4b.

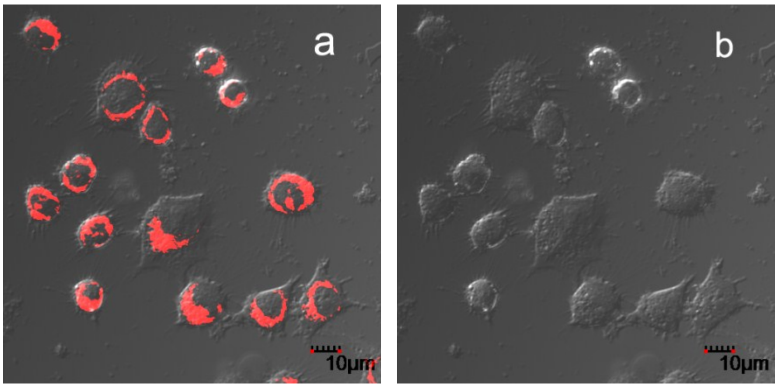


Fig. S12 (a) Merged images of brightfield (b) and red channel (Fig. 4c). (b) Brightfield images of Fig.

4c.

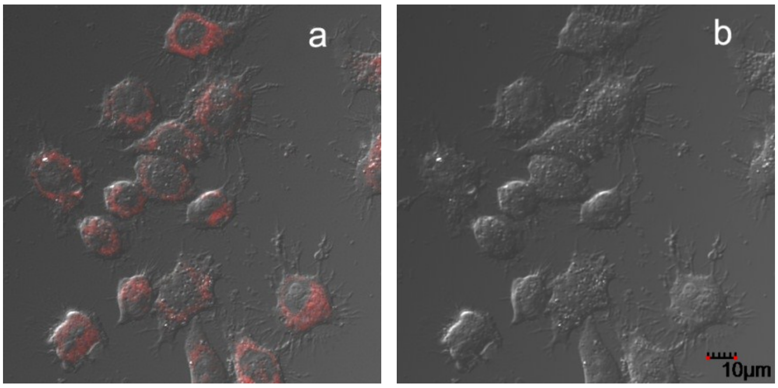


Fig. S13 (a) Merged images of brightfield (b) and red channel (Fig. 4d). (b) Brightfield images of Fig. 4d.

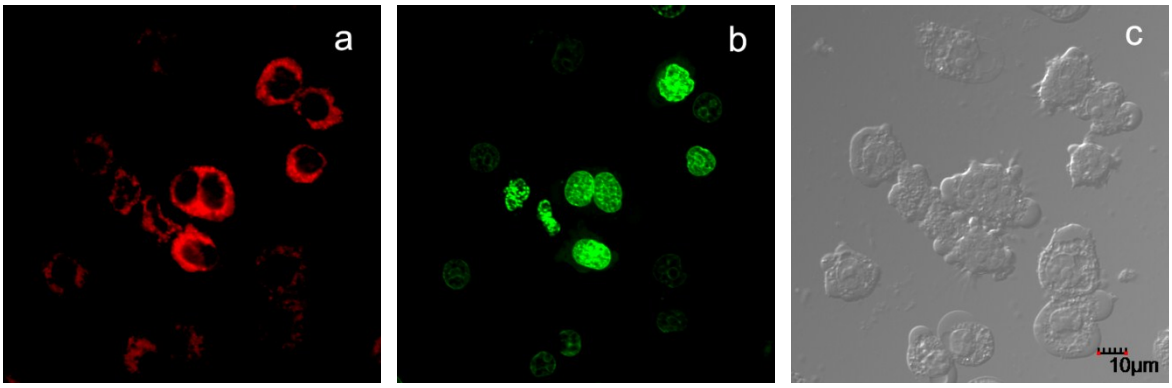


Fig. S14 (a) Red channel of Fig. 4e. (b) Green channel of Fig. 4e. (c) Brightfield images of Fig. 4e.

8. Theoretical and Computational Methods

Our data suggested that the detection mechanism relied on photoinduced electron transfer process from the excited fluorophore to the oxoammonium cation moiety (donor-excited PET, d-PET).[16] The mechanism was proved to be effective via the density functional theory calculations of mCy-TemOH and mCy-Oam (Fig.S13), Cy-TemOH and Cy-Oam (Fig. S14) (BP86 functional with TZVP basis sets using Gaussian 09 package).[17] Here, excitation energies and oscillator strengths (*f*) were defined to evaluate electronic excited states and photophysical properties of the probe (Table S1). mCy-TemOH shows the strongest absorption spectra around 498 nm in $S_0 \rightarrow S_1$ with largest oscillator strength by 1.9721, and the electron transition for H→L is the localized excited state over the conjugated organic chain in the middle of the molecule. In addition, the electron relaxation form L to H is also the LE state, and the large overlap of the electrons can induce strong fluorescence emission, which is in good agreement with the experimental results. mCy-Oam shows the $S_0 \rightarrow S_1$ transition around 494 nm with the largest oscillator strength by 1.9147, in which the H→L+1 transition is the LE state over the conjugated chain. It is obvious from Fig. S13 that the LUMO orbital of ring including the oxoammonium cation is between the HOMO and LUMO (L+1) of the organic conjugated chain, so the electron relaxation form L+1 to L and finally back to H is the distinct photoinduced electron transition character, which can be applied to explaining the fluorescence quenching effect for mCy-Oam. The main absorption spectrum for Cy-TemOH locates around 537 nm with the LE state transition of H→L, where the electrons delocalize over the organic conjugated chain in the Cy moiety. In addition, the electron relaxation for L→H from S_1 to S_0 state is the LE state with the totally overlapping electron over the organic conjugated chain in the Cy segment, responsible to the strong fluorescence emission. The dark S_1 state around 585 nm for Cy-Oam shows the electron transition of H→L with large charge transfer from Cy moiety to the oxoammonium cation. The main absorption around 550 nm exhibits in $S_0 \rightarrow S_2$ with largest oscillator strength of 2.1692, and the electron transition for H→L+1 shows the LE character over the Cy moiety. Similar with mCy-Oam, the LUMO orbital for oxoammonium cation is localized between the HOMO and LUMO (L+1) of the Cy moiety. However, the electron relaxations in both $S_2 \rightarrow S_1$ and $S_1 \rightarrow S_0$ are the typical charge transfer by photoinduced electron transition from oxoammonium cation to Cy moiety, which can induce the fluorescence quenching effect.

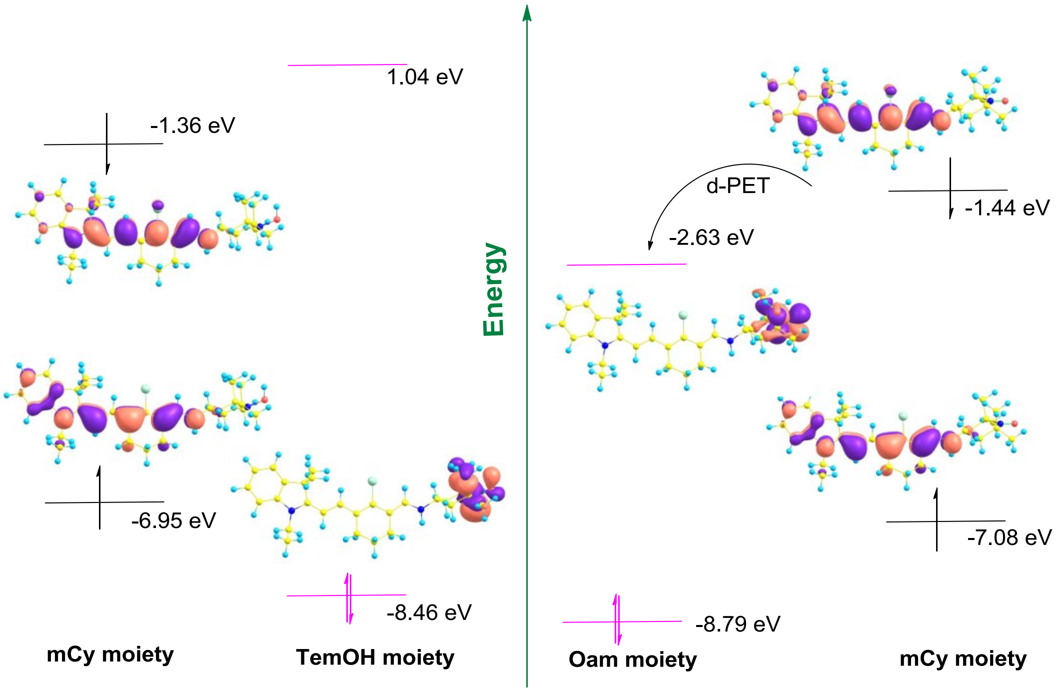


Fig. S15 Frontier molecular orbital energy illustrations show the relative energetic dispositions of the orbitals of two moieties in mCy-TemOH and mCy-Oam.

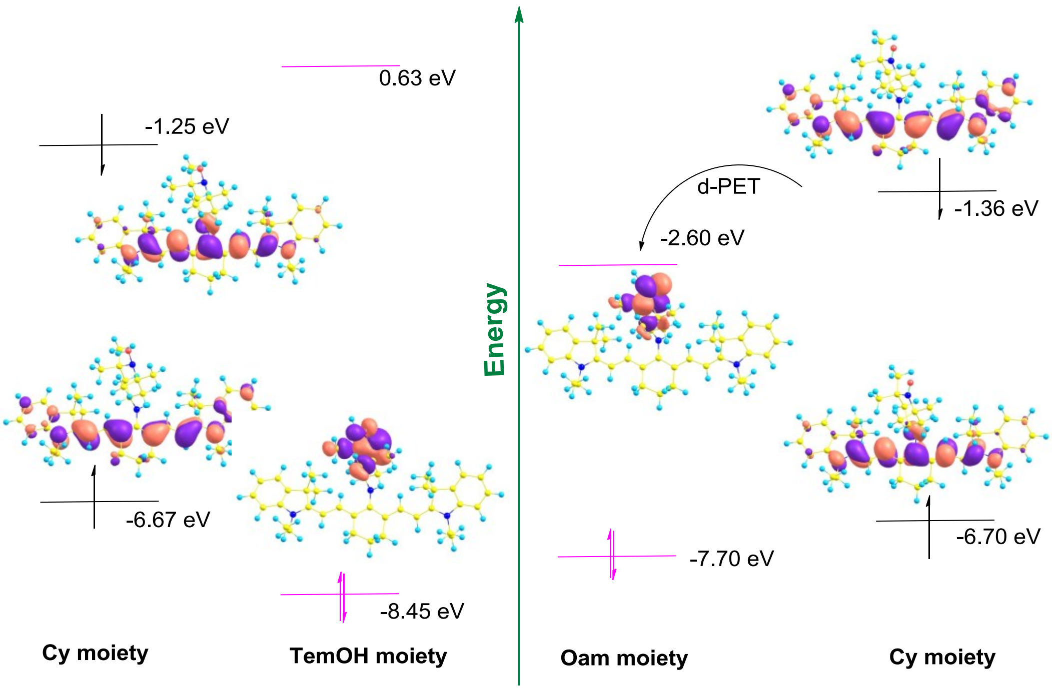


Fig. S16 Frontier molecular orbital energy illustrations show the relative energetic dispositions of the orbitals of two moieties in Cy-TemOH and Cy-Oam.

Table S1. Calculated electronic transitions energies for the compounds at TD-DFT/wB97XD/TZVP level with COSMO solvation model

	Exp.(nm)	Cal.	State	*f*	Transition	CI
***m*Cy-TemOH**	610	498	$S_0 \rightarrow S_1$	1.9721	H→L	0.69
***m*Cy-Oam**	610	494	$S_0 \rightarrow S_1$	1.9147	H→L+1	0.69
Cy-TemOH	702	537	$S_0 \rightarrow S_1$	2.1707	H→L	0.68
Cy-Oam	702	585	$S_0 \rightarrow S_1$	0.0336	H→L	0.70
		550	$S_0 \rightarrow S_2$	2.1692	H→L+1	0.68

[16] A. P. de Silva, H. Q. Gunaratne, T. Gunnlaugsson, A. J. Huxley, C. P. McCoy, J. T. Rademacher, T. E. Rice, *Chem. Rev.* **1997**, 97, 1515. (b) T. Ueno, Y. Urano, K. Setsukinai, H. Takakusa, H. Kojima, K. Kikuchi, K. Ohkubo, S. Fukuzumi, T. Nagano, *J. Am. Chem. Soc.* **2004**, 126, 14079.

[17] The Gaussian 09 package refer to Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Nor-mand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**

Computational method:

In order to investigate the fluorescence mechanism, density functional theory (DFT) and time-dependent density functional theory (TD-DFT) methods have been carries out to study the ground state structure and electron transition for the four compounds mCy-TemOH, Cy-TemOH, mCy-Oam, and Cy-Oam, and the latter method has been confirmed to be an effective one to carry out the electron transition. Herein, the latest functional wB97XD[18] from Head-Gordon and coworkers, which includes empirical dispersion and long range correction, has been used with the triple-ζ valence quality with one set of polarization functions (TZVP)[19] to be an appropriate basis set for such ionic organic compounds.[20] In order to be in good agreement with the experimental spectra, the solvent effect in aqueous solution was employed in the SCRF calculations by using the conductor-like screening model (COSMO) method.[21] The geometries for the four compounds were fully optimized without symmetry constraints, and all the local minima were confirmed by the absence of an imaginary mode in vibrational analysis calculations.

[18] J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615-6620.
[19] O. Treutler, R.Ahlrichs, *J. Chem. Phys.* **1995**, *102*, 346 -354.
[20] S. K. Schneider, G. R. Julius, C. Loschen, H. G. Raubenheimer, G. Frenking, W. A. Herrmann, *Dalton Trans*. **2006**, 1226-1233.
[21] A. Klamt, G. Schüürmann, *J. Chem. Soc. Perkin Trans.2*, **1993**, *5*, 799.

XYZ Coordinates (angstrom) and SCF Energies (a.u.)
m**Cy-TemOH**
Energy = -1868.4787874

C	0.550723	7.453604	-2.410289
C	0.224019	6.602882	-1.370931
C	-0.318041	7.110349	-0.198657
C	-0.542251	8.464972	-0.009156
C	-0.207542	9.317405	-1.061818
C	0.329519	8.823166	-2.248656
C	0.363742	5.102431	-1.249536
C	-0.173493	4.867647	0.166368
N	-0.567488	6.043523	0.687869
C	-1.115720	6.245109	2.025567
C	1.846260	4.705774	-1.365859
C	-0.497657	4.405342	-2.318544
C	-0.251632	3.673439	0.877707
H	0.974859	7.067009	-3.331802
H	-0.951777	8.861585	0.912548
H	-0.368094	10.384099	-0.947100
H	0.582592	9.508455	-3.050468
H	-1.782327	7.106433	1.977204
H	-1.740564	5.387027	2.273894
H	2.442593	5.201660	-0.596238

H	1.988805	3.628456	-1.271906
H	2.223351	5.013425	-2.344177
H	-1.553320	4.657703	-2.194783
H	-0.394923	3.319959	-2.285395
H	-0.176918	4.741336	-3.307456
C	0.136161	-1.260728	1.017894
C	0.087925	2.427153	0.356965
H	0.401166	2.381662	-0.675808
C	0.276263	-0.009046	0.406474
C	0.030418	1.218075	1.046809
C	-0.364916	1.179691	2.508918
C	-0.208819	-1.321719	2.490165
H	0.002418	2.078599	3.009714
H	-1.458879	1.198523	2.597084
C	0.191743	-0.046770	3.217296
H	-1.284431	-1.502364	2.613099
H	0.304787	-2.169951	2.954837
H	1.284624	0.021971	3.255046
H	-0.165289	-0.079168	4.249498
C	-0.022505	6.458754	3.063873
H	-0.608368	3.726411	1.898069
H	-0.473618	6.608055	4.047206
H	0.575404	7.340870	2.822255
H	0.642383	5.593412	3.117758
Cl	0.754505	0.025692	-1.290285
C	0.245408	-2.444123	0.287231
H	0.512025	-2.423168	-0.762885
N	0.027565	-3.646774	0.775991
H	-0.252094	-3.747362	1.743967
C	0.147708	-4.886673	0.014565
C	1.189619	-5.791136	0.662286
C	-1.197116	-5.602633	-0.028899
H	0.460822	-4.598727	-0.990893
C	1.329357	-7.149361	-0.040118
H	0.897315	-5.960542	1.705150
H	2.164547	-5.296269	0.671518
C	-1.135219	-6.952951	-0.757222
H	-1.530817	-5.771205	1.001510
H	-1.944438	-4.971371	-0.517542
C	-1.032808	-6.742252	-2.280296
H	-0.864447	-7.683588	-2.810831
H	-1.980170	-6.338461	-2.646385
H	-0.249695	-6.043901	-2.572074
C	-2.439999	-7.703542	-0.467633

H	-2.495693	-8.636697	-1.030735
H	-2.523199	-7.933565	0.597588
H	-3.293241	-7.083221	-0.755255
C	2.090153	-6.992617	-1.371171
H	3.131097	-6.739674	-1.154372
H	2.106214	-7.923500	-1.944705
H	1.693294	-6.206776	-2.012291
C	2.151045	-8.068722	0.870502
H	1.620090	-8.257643	1.806904
H	2.355046	-9.025735	0.387312
H	3.108616	-7.595613	1.104194
N	-0.032310	-7.730794	-0.139546
O	0.023026	-9.031403	-0.682484
H	0.286608	-8.976311	-1.611737

***m*Cy-Oam**

Energy = -1867.6794279

C	0.402841	7.397234	-2.441940
C	0.140273	6.552129	-1.379598
C	-0.338633	7.065823	-0.183874
C	-0.562230	8.419336	0.010803
C	-0.292726	9.265788	-1.064558
C	0.181553	8.765704	-2.275976
C	0.293614	5.054205	-1.254373
C	-0.161211	4.830291	0.189947
N	-0.529243	6.001160	0.723898
C	-1.011332	6.212077	2.087390
C	1.768333	4.661041	-1.453187
C	-0.628392	4.344546	-2.263558
C	-0.198396	3.634386	0.917328
H	0.777760	7.007012	-3.382960
H	-0.922814	8.819333	0.951251
H	-0.454081	10.332163	-0.949135
H	0.384387	9.447287	-3.095029
H	-1.687772	7.066370	2.061117
H	-1.614074	5.350974	2.375250
H	2.408006	5.171540	-0.729474
H	1.921956	3.585961	-1.352314
H	2.082174	4.954996	-2.457561
H	-1.675460	4.597098	-2.081098
H	-0.521910	3.259816	-2.224913
H	-0.366447	4.671010	-3.272582
C	0.111135	-1.301622	1.064373
C	0.109392	2.394187	0.387177

H	0.375822	2.340882	-0.658185
C	0.272173	-0.042081	0.447457
C	0.070756	1.179545	1.089213
C	-0.262483	1.164191	2.567159
C	-0.231057	-1.342787	2.537993
H	0.180952	2.040385	3.047198
H	-1.348194	1.253088	2.700954
C	0.248424	-0.091139	3.258452
H	-1.314781	-1.459005	2.667044
H	0.234394	-2.218328	3.002157
H	1.344019	-0.078142	3.269866
H	-0.084566	-0.107722	4.299018
C	0.131909	6.448229	3.064535
H	-0.496149	3.696645	1.955767
H	-0.271821	6.606547	4.066722
H	0.709218	7.332079	2.782696
H	0.805878	5.588893	3.096302
Cl	0.716154	-0.024085	-1.258930
C	0.195766	-2.476750	0.338691
H	0.461877	-2.460019	-0.711402
N	-0.040923	-3.688212	0.826534
H	-0.343767	-3.791627	1.786378
C	0.040539	-4.908042	0.040222
C	0.947822	-5.906966	0.748891
C	-1.349089	-5.513634	-0.126697
H	0.457506	-4.626362	-0.927644
C	1.097823	-7.253308	0.031664
H	0.551985	-6.087129	1.753623
H	1.953376	-5.496089	0.860484
C	-1.372986	-6.815530	-0.934712
H	-1.774691	-5.701464	0.864157
H	-2.009939	-4.813274	-0.642047
C	-1.084435	-6.594081	-2.432081
H	-0.922191	-7.544822	-2.942061
H	-1.979213	-6.126740	-2.846500
H	-0.243244	-5.931311	-2.620385
C	-2.704124	-7.535318	-0.761934
H	-2.785829	-8.404309	-1.414320
H	-2.858323	-7.840076	0.274897
H	-3.487247	-6.826130	-1.034266
C	1.960146	-7.164519	-1.242269
H	2.987314	-7.020529	-0.903154
H	1.908444	-8.095338	-1.809000
H	1.700370	-6.330111	-1.889099

C	1.671134	-8.303515	0.974785
H	0.989727	-8.504136	1.803665
H	1.900567	-9.234775	0.457726
H	2.598732	-7.896922	1.380693
N	-0.276593	-7.739617	-0.416127
O	-0.488682	-8.896684	-0.395936

Cy-TemOH

E= -1968.0090336

C	0.445737	7.454789	-1.880973
C	-0.283794	6.582123	-1.096434
C	-1.198375	7.070305	-0.172230
C	-1.407731	8.428375	0.014005
C	-0.665892	9.303312	-0.781216
C	0.247810	8.828686	-1.719213
C	-0.264524	5.071454	-1.029868
C	-1.309186	4.803947	0.058958
N	-1.811936	5.987649	0.481900
C	-2.807905	6.161215	1.531251
C	1.127664	4.589853	-0.591714
C	-0.668401	4.469812	-2.386969
C	1.389238	-7.496611	-0.446133
C	0.284090	-6.670315	-0.378541
C	-0.996354	-7.209201	-0.410678
C	-1.218356	-8.573262	-0.529241
C	-0.096172	-9.401013	-0.600482
C	1.192891	-8.876092	-0.556543
C	0.192778	-5.164239	-0.264435
C	-1.329702	-4.954354	-0.265889
N	-1.935332	-6.171405	-0.309796
C	-3.373171	-6.398688	-0.329106
C	0.890544	-4.510267	-1.470189
C	0.814657	-4.702880	1.066243
C	-2.035111	-3.772433	-0.212178
C	-1.431897	-2.496693	-0.163944
C	-1.715130	3.590936	0.585081
H	1.162588	7.082774	-2.606616
H	-2.108969	8.809375	0.747367
H	-0.805802	10.372275	-0.659389
H	0.813028	9.529214	-2.324571
H	-3.353751	7.080064	1.314913
H	-3.532177	5.349195	1.456119
H	1.414431	5.035307	0.363952
H	1.163646	3.506975	-0.485203

H	1.866700	4.880066	-1.342579
H	-1.676967	4.782102	-2.668275
H	-0.634147	3.379347	-2.376058
H	0.027067	4.819136	-3.154097
H	2.392840	-7.083053	-0.415912
H	-2.216189	-8.993970	-0.575022
H	-0.237635	-10.472495	-0.696372
H	2.048205	-9.541015	-0.612276
H	-3.843981	-5.678980	0.342588
H	-3.554015	-7.383602	0.103088
H	0.398385	-4.789414	-2.404807
H	0.910916	-3.422100	-1.401611
H	1.926903	-4.854283	-1.512896
H	0.711339	-3.627073	1.210567
H	0.342292	-5.208854	1.911867
H	1.880795	-4.943851	1.071961
H	-3.116918	-3.829502	-0.218956
C	-2.047982	-1.279928	0.010787
C	-1.270635	2.333120	0.145126
H	-0.354220	-2.478018	-0.246194
H	-0.508510	2.291999	-0.622863
C	-1.258445	-0.080328	0.007964
C	-1.781302	1.119648	0.567682
C	-2.984688	1.080033	1.487395
C	-3.494915	-1.123306	0.402323
H	-2.733265	1.536935	2.451434
H	-3.769287	1.712577	1.053437
C	-3.547584	-0.322381	1.705316
H	-4.056414	-0.593941	-0.377768
H	-3.973847	-2.093962	0.535961
H	-2.965964	-0.854513	2.466218
H	-4.573175	-0.251259	2.077679
C	-3.956149	-6.308605	-1.733390
C	-2.176968	6.217685	2.916408
H	-2.441839	3.613514	1.388111
H	-5.033244	-6.488393	-1.700125
H	-3.503293	-7.056356	-2.389372
H	-3.786999	-5.320206	-2.167482
H	-2.951944	6.363182	3.672368
H	-1.468531	7.046924	2.985477
H	-1.646581	5.289543	3.143022
N	-0.027806	-0.075342	-0.592325
H	0.128186	-0.860278	-1.210516
C	1.210984	0.311106	0.103659

C	1.718337	-0.876059	0.916725
C	2.269650	0.711419	-0.911710
H	0.973360	1.147739	0.760101
C	3.060297	-0.629198	1.612825
H	1.839998	-1.724122	0.232650
H	0.976193	-1.165770	1.667250
C	3.643058	1.004015	-0.285335
H	2.383410	-0.110090	-1.629751
H	1.944067	1.589105	-1.477789
C	3.579837	-1.977944	2.124084
H	2.831076	-2.438709	2.774185
H	3.774698	-2.656463	1.289444
H	4.500641	-1.858345	2.697903
C	2.880508	0.306438	2.823054
H	2.300453	-0.215824	3.588355
H	3.838305	0.571661	3.279512
H	2.350865	1.228039	2.585801
C	4.672178	1.068948	-1.419822
H	4.348405	1.797033	-2.168522
H	5.652254	1.376899	-1.050875
H	4.773188	0.094468	-1.904401
C	3.641563	2.367867	0.431284
H	4.553499	2.522501	1.014988
H	3.612246	3.161835	-0.318064
H	2.787638	2.513907	1.091295
N	4.000906	-0.159395	0.565936
O	5.297454	0.000002	1.099911
H	5.293607	0.739363	1.724181

Cy-Oam

E= -1967.2108256

C	-0.061066	7.406694	-2.260118
C	-0.589053	6.547846	-1.314810
C	-1.290389	7.051345	-0.227107
C	-1.475415	8.411504	-0.032293
C	-0.937728	9.272305	-0.990278
C	-0.242145	8.781976	-2.093033
C	-0.532778	5.040378	-1.217359
C	-1.317814	4.791476	0.074273
N	-1.733136	5.979060	0.568785
C	-2.483597	6.169367	1.804148
C	0.928042	4.584205	-1.074336
C	-1.208302	4.396148	-2.439681
C	1.458792	-7.508959	-0.484739

C	0.374432	-6.688981	-0.238250
C	-0.881765	-7.237454	-0.011095
C	-1.103082	-8.606497	-0.037345
C	-0.002778	-9.428048	-0.289787
C	1.264118	-8.892652	-0.508077
C	0.285788	-5.180595	-0.159671
C	-1.213198	-4.981747	0.110652
N	-1.799568	-6.201695	0.226357
C	-3.214426	-6.438278	0.477662
C	0.744548	-4.565558	-1.493646
C	1.131842	-4.672105	1.022230
C	-1.914096	-3.802167	0.248525
C	-1.332420	-2.522973	0.137865
C	-1.595087	3.586762	0.699162
H	0.485006	7.021501	-3.115881
H	-2.005922	8.806684	0.826168
H	-1.066044	10.342513	-0.867219
H	0.163917	9.472755	-2.824191
H	-3.045361	7.097959	1.703107
H	-3.222194	5.370672	1.884475
H	1.404060	5.055341	-0.210992
H	0.998333	3.504748	-0.952734
H	1.486395	4.861540	-1.971885
H	-2.255469	4.699259	-2.512715
H	-1.165754	3.306643	-2.400983
H	-0.692578	4.721437	-3.346517
H	2.444197	-7.087262	-0.658356
H	-2.085223	-9.036775	0.120324
H	-0.144529	-10.503416	-0.319117
H	2.102404	-9.553112	-0.702504
H	-3.567571	-5.688575	1.187255
H	-3.301804	-7.401437	0.981796
H	0.100333	-4.890657	-2.313963
H	0.752919	-3.475143	-1.472933
H	1.763956	-4.896761	-1.705921
H	1.031646	-3.595186	1.160850
H	0.834044	-5.164495	1.951195
H	2.185766	-4.894326	0.836641
H	-2.977104	-3.867980	0.444777
C	-1.928768	-1.305506	0.378126
C	-1.219949	2.322289	0.223251
H	-0.288827	-2.497724	-0.142072
H	-0.607474	2.259913	-0.668330
C	-1.183746	-0.096769	0.189803

C	-1.628778	1.118346	0.774285
C	-2.651873	1.104054	1.892412
C	-3.289249	-1.153250	1.007453
H	-2.242718	1.604954	2.777257
H	-3.512741	1.707133	1.577783
C	-3.138236	-0.294727	2.264605
H	-3.987483	-0.668765	0.313385
H	-3.717366	-2.123457	1.261414
H	-2.424470	-0.781908	2.937875
H	-4.087902	-0.221155	2.801199
C	-4.038635	-6.420399	-0.803277
C	-1.575789	6.214739	3.026078
H	-2.152149	3.625839	1.627221
H	-5.090141	-6.606271	-0.572851
H	-3.696581	-7.194274	-1.494994
H	-3.963192	-5.452044	-1.303806
H	-2.173068	6.378621	3.925759
H	-0.852389	7.029420	2.940891
H	-1.028520	5.276623	3.144653
N	-0.067099	-0.099903	-0.615941
H	-0.002105	-0.908222	-1.220383
C	1.250691	0.332502	-0.143770
C	1.914083	-0.811860	0.619728
C	2.115977	0.702126	-1.339549
H	1.106105	1.193693	0.506807
C	3.324747	-0.519282	1.135322
H	1.962693	-1.685883	-0.038820
H	1.314037	-1.090025	1.490139
C	3.551278	1.111942	-0.984047
H	2.157421	-0.152257	-2.023808
H	1.676147	1.536050	-1.890701
C	4.024896	-1.805743	1.552484
H	3.381671	-2.296850	2.284394
H	4.154840	-2.479551	0.703336
H	4.991513	-1.613846	2.017863
C	3.337377	0.494132	2.294062
H	2.937071	-0.032216	3.162034
H	4.355213	0.814623	2.521466
H	2.713830	1.366138	2.113804
C	4.436299	1.109726	-2.222594
H	3.955383	1.755444	-2.959201
H	5.429241	1.508028	-2.015129
H	4.525979	0.108065	-2.647036
C	3.637574	2.481219	-0.282287

H	4.624796	2.631662	0.157578
H	3.489089	3.232882	-1.058632
H	2.874107	2.627315	0.477981
N	4.129574	0.098802	-0.001412
O	5.264269	-0.193977	-0.106316

Vibrational frequencies for the compounds respectively.

***m*Cy-TemOH**

mode	wave number cm^{-1}	IR intensity km/mol	selection rules IR
1	9.7787	1.6031	YES
2	17.9777	0.1586	YES
3	23.3629	2.1868	YES
4	27.6950	1.2218	YES
5	40.6757	1.8993	YES
6	51.5148	3.5726	YES
7	56.0813	3.2241	YES
8	79.8731	1.8868	YES
9	86.1706	2.2781	YES
10	91.3519	4.3847	YES
11	107.2275	2.1384	YES
12	112.1778	0.5935	YES
13	126.1900	12.1823	YES
14	131.9065	0.6425	YES
15	134.2850	0.8361	YES
16	148.4130	1.3895	YES
17	170.9286	1.5003	YES
18	176.4665	16.9775	YES
19	197.2559	6.2574	YES
20	200.0358	36.8183	YES
21	205.7110	0.9917	YES
22	217.4658	10.4930	YES
23	240.2190	1.9075	YES
24	246.3241	3.5732	YES
25	247.7145	0.8086	YES
26	253.1389	1.0442	YES
27	256.1751	10.2651	YES
28	265.7254	3.0572	YES
29	275.6260	2.3100	YES
30	277.6474	1.5233	YES
31	287.0552	6.3525	YES
32	290.3521	2.9648	YES
33	302.9454	33.9693	YES

34	308.8062	149.9338	YES
35	313.1319	2.6386	YES
36	316.8103	56.2242	YES
37	332.3205	3.9328	YES
38	341.7939	17.7232	YES
39	361.7832	2.2457	YES
40	364.7591	11.5437	YES
41	376.5762	47.8962	YES
42	383.5419	24.4740	YES
43	385.7838	14.3426	YES
44	393.5641	0.5570	YES
45	408.9767	2.3274	YES
46	429.5605	150.1453	YES
47	429.9607	103.1414	YES
48	443.1649	28.7371	YES
49	450.8584	28.0554	YES
50	466.8038	68.3465	YES
51	477.9037	84.7863	YES
52	483.8032	119.5467	YES
53	490.6459	340.9755	YES
54	496.0860	121.7572	YES
55	518.3577	192.9602	YES
56	536.0154	78.1461	YES
57	551.6704	20.1359	YES
58	565.7688	85.1958	YES
59	571.8772	6.2284	YES
60	581.7133	115.1373	YES
61	586.4281	41.9889	YES
62	596.7554	6.2909	YES
63	616.4960	189.2705	YES
64	636.5248	26.6006	YES
65	657.2153	142.7817	YES
66	666.0056	52.8316	YES
67	699.4000	19.8493	YES
68	716.7218	729.4951	YES
69	724.3208	143.3286	YES
70	733.6395	583.5113	YES
71	760.7915	81.5485	YES
72	778.9980	136.5452	YES
73	788.3350	240.8823	YES
74	790.4548	1321.3690	YES
75	818.1526	2.6477	YES
76	823.5639	1021.6925	YES
77	837.0145	693.8986	YES

78	846.4911	559.8509	YES
79	865.1762	25.7506	YES
80	871.7618	7.0999	YES
81	883.5171	48.2535	YES
82	886.7835	1133.8741	YES
83	896.5385	19.2320	YES
84	914.5742	1626.3165	YES
85	937.4840	927.2279	YES
86	947.5726	12.5873	YES
87	952.2323	5383.6038	YES
88	956.9192	180.0591	YES
89	964.2421	143.2154	YES
90	967.5456	24.4283	YES
91	967.8720	1192.7689	YES
92	969.7345	1045.3698	YES
93	978.9075	71.6781	YES
94	981.8818	636.3691	YES
95	995.4480	930.6518	YES
96	1002.0354	7166.9525	YES
97	1010.6951	455.8072	YES
98	1021.4113	10.6439	YES
99	1021.8053	17.2386	YES
100	1027.0060	10.9069	YES
101	1033.7612	16305.3899	YES
102	1050.1177	17.2619	YES
103	1051.6355	821.8879	YES
104	1062.0225	2619.8940	YES
105	1081.8225	0.2891	YES
106	1086.4701	655.4249	YES
107	1088.7647	374.1561	YES
108	1099.8045	1355.6178	YES
109	1103.6855	698.4054	YES
110	1117.6489	358.7804	YES
111	1119.9342	7.6200	YES
112	1123.8723	135.9870	YES
113	1136.2357	1744.2478	YES
114	1151.9861	7.5396	YES
115	1155.7270	148.9651	YES
116	1181.8836	1312.7647	YES
117	1184.2296	475.6869	YES
118	1188.6632	469.3740	YES
119	1198.2170	29.1982	YES
120	1216.2423	119.2879	YES
121	1217.5879	43.3254	YES

122	1224.8586	39.3324	YES
123	1241.8280	13.4367	YES
124	1256.7774	672.5514	YES
125	1261.4718	23.2521	YES
126	1274.6064	1939.6217	YES
127	1292.7957	28.8140	YES
128	1298.6180	36.8496	YES
129	1302.7116	46.7778	YES
130	1306.8562	5.3752	YES
131	1318.4061	7.2750	YES
132	1325.9998	6.5582	YES
133	1330.9261	37.9791	YES
134	1340.4841	94.1041	YES
135	1347.8299	6.7813	YES
136	1351.3601	18.6351	YES
137	1358.8193	13.4270	YES
138	1376.1247	79.4943	YES
139	1378.4272	175.1704	YES
140	1394.2628	49.5979	YES
141	1399.2708	285.3062	YES
142	1401.0770	415.3659	YES
143	1402.3226	78.1429	YES
144	1411.0845	12.2592	YES
145	1411.9418	27.5985	YES
146	1416.0050	16.9661	YES
147	1420.4629	5.6688	YES
148	1423.0950	188.2632	YES
149	1426.3082	16.3954	YES
150	1429.7234	28.4944	YES
151	1432.2639	532.2387	YES
152	1434.4893	12.2210	YES
153	1441.1564	296.7763	YES
154	1447.0968	105.5777	YES
155	1458.1750	155.1995	YES
156	1460.2446	77.0633	YES
157	1476.7953	4.2032	YES
158	1478.9846	47.1563	YES
159	1486.2472	783.4160	YES
160	1487.6967	1.1022	YES
161	1488.7359	6.4991	YES
162	1490.6489	324.1387	YES
163	1491.1940	8.1954	YES
164	1492.2631	53.6788	YES
165	1492.7547	658.6484	YES

166	1495.7868	211.0351	YES
167	1499.2173	2.2368	YES
168	1500.4949	159.8404	YES
169	1500.7204	9.8502	YES
170	1502.1837	51.7173	YES
171	1502.6712	32.9898	YES
172	1505.3263	47.2215	YES
173	1513.1431	17.6109	YES
174	1516.3839	10.4359	YES
175	1517.5362	139.5389	YES
176	1520.1195	4.9725	YES
177	1526.8772	304.0441	YES
178	1539.5017	92.4433	YES
179	1540.2811	47.2757	YES
180	1547.1493	23.7451	YES
181	1597.2691	99.6380	YES
182	1624.9459	1388.9558	YES
183	1677.8226	17.8737	YES
184	1690.4897	65.0443	YES
185	1704.8926	469.3524	YES
186	3036.7021	63.3877	YES
187	3037.9599	57.4840	YES
188	3053.2626	12.0648	YES
189	3054.3940	9.4639	YES
190	3055.1979	30.0006	YES
191	3055.7964	47.5159	YES
192	3056.2777	30.3405	YES
193	3058.1423	125.7345	YES
194	3062.1457	37.6005	YES
195	3063.8741	38.8832	YES
196	3064.7813	19.5911	YES
197	3067.8184	23.5639	YES
198	3086.2265	71.3564	YES
199	3108.5147	38.3268	YES
200	3111.0461	53.8408	YES
201	3112.3068	9.0697	YES
202	3115.2401	77.7233	YES
203	3116.4623	23.7819	YES
204	3122.9084	21.6899	YES
205	3124.3961	38.2965	YES
206	3129.8243	71.7643	YES
207	3130.3919	19.3184	YES
208	3131.8616	44.2171	YES
209	3133.5495	92.2526	YES

210	3139.0043	55.4164	YES
211	3140.2486	21.4831	YES
212	3142.4014	44.9294	YES
213	3145.5634	6.8877	YES
214	3145.8633	104.3975	YES
215	3151.9365	34.6654	YES
216	3155.6096	52.8396	YES
217	3157.8238	39.8344	YES
218	3161.0839	30.8527	YES
219	3178.3950	65.1159	YES
220	3197.8750	3.0395	YES
221	3205.7884	11.9899	YES
222	3219.7418	28.9010	YES
223	3227.7893	27.9317	YES
224	3235.0704	3.2209	YES
225	3235.4467	6.9409	YES
226	3273.3973	1.6924	YES
227	3616.5758	473.7701	YES
228	3735.1788	9.7686	YES

***m*Cy-Oam**

mode	wave number cm^{-1}	IR intensity km/mol	selection rules IR
1	18.0331	0.7951	YES
2	21.8443	0.1546	YES
3	28.5785	1.6002	YES
4	30.9451	0.3339	YES
5	39.7471	1.5563	YES
6	50.1543	2.3867	YES
7	54.6735	2.1337	YES
8	70.2354	2.2665	YES
9	77.0434	4.5044	YES
10	82.3176	0.4286	YES
11	97.6805	1.4043	YES
12	107.2537	0.0469	YES
13	120.7440	2.6730	YES
14	126.5169	0.9802	YES
15	132.4238	1.7954	YES
16	145.1285	7.7051	YES
17	171.7935	2.9030	YES
18	175.1267	10.1022	YES
19	193.5479	3.6596	YES
20	197.4076	13.9935	YES
21	203.0713	2.6292	YES

22	223.6316	4.8797	YES
23	229.7113	3.8605	YES
24	241.4589	3.2509	YES
25	250.2714	0.4530	YES
26	256.8892	5.1944	YES
27	265.5158	0.6579	YES
28	276.8441	0.6317	YES
29	279.8072	0.2054	YES
30	283.4309	0.4932	YES
31	291.9828	6.2591	YES
32	299.1730	0.2923	YES
33	300.9386	1.0253	YES
34	302.9688	57.1403	YES
35	309.3978	53.4960	YES
36	314.0024	4.0227	YES
37	321.0623	56.6125	YES
38	345.4500	1.0035	YES
39	359.3362	22.3512	YES
40	362.1380	19.4945	YES
41	366.8997	0.8733	YES
42	382.7523	16.0709	YES
43	385.1477	1.4383	YES
44	401.6720	23.7725	YES
45	417.9074	6.3296	YES
46	425.4910	202.4366	YES
47	429.8739	3.6464	YES
48	440.3397	50.7995	YES
49	442.4053	26.3026	YES
50	465.8282	31.7673	YES
51	475.7564	6.5272	YES
52	485.8268	277.5184	YES
53	494.9449	9.5962	YES
54	513.0002	325.8147	YES
55	532.9984	1.0898	YES
56	550.4116	29.2455	YES
57	566.0043	37.4206	YES
58	567.2932	26.2352	YES
59	577.0635	35.7666	YES
60	590.0748	14.1257	YES
61	597.3975	6.8490	YES
62	631.7116	37.5086	YES
63	649.1824	225.4713	YES
64	651.7547	489.4288	YES
65	675.1604	416.2397	YES

66	688.5666	94.4445	YES
67	727.3744	31.8163	YES
68	732.3192	474.5931	YES
69	755.3969	159.1215	YES
70	765.3576	27.3609	YES
71	775.8742	122.6128	YES
72	788.2048	106.7932	YES
73	792.6267	1168.1081	YES
74	825.4623	759.0435	YES
75	827.6114	3.1381	YES
76	837.0966	416.5016	YES
77	851.8908	435.2958	YES
78	854.3407	197.6737	YES
79	866.6739	14.4783	YES
80	891.2572	104.0907	YES
81	891.5093	482.3507	YES
82	892.0466	84.0791	YES
83	916.8737	904.6164	YES
84	934.7750	21.0311	YES
85	937.6958	184.9728	YES
86	954.5010	3477.2316	YES
87	966.2961	1222.6817	YES
88	967.6193	561.0883	YES
89	970.7136	430.7926	YES
90	975.1297	30.6327	YES
91	977.1658	31.9559	YES
92	979.3175	7.7185	YES
93	980.5844	5.1507	YES
94	982.4131	18.7549	YES
95	994.5158	1173.2573	YES
96	1008.1345	5050.2837	YES
97	1016.2016	106.2110	YES
98	1020.4645	3.1119	YES
99	1039.0789	17272.8285	YES
100	1042.8903	13.8447	YES
101	1051.9435	737.0646	YES
102	1060.1558	1.2683	YES
103	1062.6900	4283.7453	YES
104	1084.7865	277.6188	YES
105	1088.8582	1434.5128	YES
106	1091.2149	472.8109	YES
107	1104.0214	1878.6812	YES
108	1116.2759	444.7476	YES
109	1128.8601	44.1257	YES

110	1132.2656	792.6251	YES
111	1139.6589	516.0135	YES
112	1145.6836	1243.9210	YES
113	1155.4787	253.0275	YES
114	1180.7913	387.4640	YES
115	1183.2581	740.8116	YES
116	1186.0831	111.7493	YES
117	1189.4851	1292.5988	YES
118	1202.2207	179.3321	YES
119	1202.8165	94.6449	YES
120	1217.7060	228.6040	YES
121	1243.4518	33.3506	YES
122	1258.2884	11.9870	YES
123	1261.3648	342.8983	YES
124	1269.9498	9.8370	YES
125	1273.3178	1848.7747	YES
126	1286.6733	13.8285	YES
127	1300.1439	173.6299	YES
128	1307.8126	25.9799	YES
129	1322.8966	38.7216	YES
130	1328.4731	12.8158	YES
131	1333.0740	27.8611	YES
132	1344.8027	5.3698	YES
133	1348.1811	12.9428	YES
134	1352.4072	19.0357	YES
135	1356.6606	41.9947	YES
136	1369.4580	233.6461	YES
137	1387.9515	13.7098	YES
138	1391.5902	11.6317	YES
139	1397.6613	660.3347	YES
140	1399.5338	102.5383	YES
141	1411.8899	4.0852	YES
142	1416.0980	152.2994	YES
143	1418.9874	18.3865	YES
144	1420.5902	55.5018	YES
145	1425.4441	21.0095	YES
146	1426.7912	31.2832	YES
147	1429.7069	127.1099	YES
148	1432.4542	99.5330	YES
149	1437.2663	142.6241	YES
150	1440.1797	541.2173	YES
151	1444.7769	77.0617	YES
152	1456.1484	53.3158	YES
153	1463.3966	45.3210	YES

154	1480.9198	672.8156	YES
155	1481.0290	680.7369	YES
156	1483.6689	14.5731	YES
157	1485.8931	526.9029	YES
158	1487.5767	12.8950	YES
159	1489.6228	86.9883	YES
160	1490.2373	311.3316	YES
161	1492.8501	23.0783	YES
162	1494.7066	4.6675	YES
163	1494.9437	31.5191	YES
164	1495.9675	18.9944	YES
165	1499.5170	23.9137	YES
166	1501.1258	25.1522	YES
167	1501.5607	94.3677	YES
168	1502.8731	91.3847	YES
169	1503.5453	13.3170	YES
170	1507.3877	66.0793	YES
171	1508.3868	96.4154	YES
172	1509.3820	1.2772	YES
173	1519.3009	28.1687	YES
174	1529.1644	30.9086	YES
175	1535.5944	391.3273	YES
176	1543.5973	67.5229	YES
177	1550.8754	17.3684	YES
178	1593.7970	151.7573	YES
179	1622.6402	1151.7304	YES
180	1678.0689	17.3333	YES
181	1691.0442	99.5603	YES
182	1701.6851	520.1011	YES
183	1789.3010	155.7017	YES
184	3034.3631	67.0321	YES
185	3036.7067	46.6104	YES
186	3057.3229	29.0079	YES
187	3057.9796	47.7499	YES
188	3063.6074	31.8305	YES
189	3066.9737	22.0905	YES
190	3072.9267	6.6183	YES
191	3075.3112	11.5555	YES
192	3078.0584	16.2266	YES
193	3079.8877	18.6067	YES
194	3084.2852	5.1297	YES
195	3087.4830	8.5956	YES
196	3090.8370	69.3413	YES
197	3104.3806	40.8559	YES

198	3113.7316	73.8125	YES
199	3115.6680	51.4233	YES
200	3129.2906	6.5990	YES
201	3132.1926	19.2089	YES
202	3137.7052	8.0221	YES
203	3142.7107	19.8381	YES
204	3143.4704	51.8263	YES
205	3144.5587	40.9822	YES
206	3145.8442	22.6465	YES
207	3153.5730	37.4246	YES
208	3159.0663	46.5066	YES
209	3162.1822	10.6675	YES
210	3163.8776	8.7358	YES
211	3165.8951	25.6943	YES
212	3166.9478	10.6824	YES
213	3167.3476	7.9187	YES
214	3174.7623	17.3526	YES
215	3175.7395	20.7778	YES
216	3194.4538	7.3942	YES
217	3195.5052	2.9618	YES
218	3205.9876	9.2190	YES
219	3206.7419	35.5670	YES
220	3218.4558	25.5156	YES
221	3227.3155	28.4000	YES
222	3236.0228	1.0832	YES
223	3237.8928	4.0520	YES
224	3272.5172	0.8203	YES
225	3621.0868	441.0585	YES

Cy-TemOH

mode	wave number	IR intensity	selection rules
	cm^{-1}	km/mol	IR
1	14.1380	0.3042	YES
2	20.3206	0.4425	YES
3	24.3369	0.5650	YES
4	25.2926	0.6122	YES
5	35.0308	0.6502	YES
6	40.0065	1.6133	YES
7	43.8916	3.9112	YES
8	50.0844	0.0480	YES
9	58.9273	9.5532	YES
10	60.4594	0.3714	YES
11	68.6835	2.4360	YES
12	69.3630	0.4896	YES

13	76.6905	1.7148	YES
14	80.9669	2.5763	YES
15	93.9806	5.8365	YES
16	100.5497	3.1442	YES
17	109.2372	3.6586	YES
18	112.2541	3.3223	YES
19	137.7345	1.2029	YES
20	138.4173	0.3480	YES
21	141.3460	12.1508	YES
22	149.1286	50.7056	YES
23	150.1966	3.9760	YES
24	160.9300	28.0311	YES
25	177.2249	10.9154	YES
26	189.8645	1.2460	YES
27	198.9320	67.6791	YES
28	208.0372	1.4091	YES
29	218.5038	8.4339	YES
30	223.4406	0.1544	YES
31	228.1609	0.2731	YES
32	234.6364	0.9527	YES
33	240.5704	10.2924	YES
34	245.5262	1.1547	YES
35	247.7621	1.9298	YES
36	257.1390	20.0327	YES
37	261.7626	4.7895	YES
38	264.3477	29.1633	YES
39	265.4042	8.6155	YES
40	271.1210	3.9386	YES
41	271.9997	28.8842	YES
42	274.3622	2.6944	YES
43	280.6107	5.5221	YES
44	282.5524	4.2984	YES
45	287.0739	3.7947	YES
46	292.7437	7.6742	YES
47	305.3133	16.0870	YES
48	311.1120	130.6599	YES
49	315.9040	279.7040	YES
50	329.2778	54.8878	YES
51	333.1594	6.3217	YES
52	343.1274	22.9169	YES
53	360.0670	19.8704	YES
54	362.2775	1.4013	YES
55	363.9022	0.3824	YES
56	366.4903	28.7504	YES

57	369.3802	70.7701	YES
58	382.6857	2.0598	YES
59	385.7529	33.3470	YES
60	412.3428	77.0624	YES
61	421.4072	7.9534	YES
62	426.7579	19.4178	YES
63	435.1875	101.1273	YES
64	444.4457	1.5728	YES
65	449.9895	33.9984	YES
66	462.8391	171.6072	YES
67	470.8845	30.4347	YES
68	481.7316	13.4642	YES
69	484.8757	2.7986	YES
70	487.9733	58.7885	YES
71	492.6927	22.1785	YES
72	497.0977	0.7591	YES
73	504.2364	2.7299	YES
74	520.3595	111.8061	YES
75	538.4179	589.4025	YES
76	552.3448	957.9643	YES
77	565.5270	24.1434	YES
78	568.4993	62.1276	YES
79	570.8892	173.9992	YES
80	581.8487	66.3888	YES
81	585.4833	24.3190	YES
82	589.6959	64.4420	YES
83	594.6918	31.3989	YES
84	597.5107	6.1762	YES
85	619.1627	9.0645	YES
86	634.0772	39.9358	YES
87	636.1939	4.3600	YES
88	650.4728	684.3140	YES
89	677.8518	84.4835	YES
90	697.5771	135.5574	YES
91	706.8994	17.8325	YES
92	717.2467	208.3096	YES
93	720.2452	163.2024	YES
94	733.5161	1395.2961	YES
95	752.3577	721.9852	YES
96	765.5498	455.0329	YES
97	767.0033	254.5286	YES
98	777.7734	1079.0119	YES
99	779.9500	173.8822	YES
100	783.8697	6.6424	YES

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101	789.3285	55.8218	YES
102	792.9603	1155.1385	YES
103	797.7468	12.3522	YES
104	822.8033	769.6322	YES
105	823.8259	690.8247	YES
106	836.4426	178.4015	YES
107	840.8944	175.9506	YES
108	851.3915	238.3207	YES
109	863.1218	142.2221	YES
110	868.5662	200.2195	YES
111	872.3448	18.8984	YES
112	878.8885	3.1866	YES
113	891.0972	2285.2965	YES
114	894.4886	195.3791	YES
115	895.6962	0.7437	YES
116	911.0138	606.1878	YES
117	925.0139	1029.1708	YES
118	937.8551	4746.9579	YES
119	944.7718	2397.0700	YES
120	947.7985	322.6979	YES
121	954.8162	256.4433	YES
122	955.6969	222.8982	YES
123	959.7815	1169.5708	YES
124	961.8060	3.3626	YES
125	964.4386	73.1445	YES
126	967.3055	35.0435	YES
127	970.7204	913.9205	YES
128	972.0884	105.4045	YES
129	974.9032	3.8358	YES
130	975.5321	55.6362	YES
131	978.6962	8.0398	YES
132	996.4415	1081.4801	YES
133	1007.3037	4987.1781	YES
134	1009.0089	0.1071	YES
135	1020.1040	33.4946	YES
136	1020.5595	7.8384	YES
137	1021.6459	388.1659	YES
138	1041.4881	14251.5905	YES
139	1049.6252	389.5928	YES
140	1054.5016	403.5934	YES
141	1056.0177	51.1703	YES
142	1056.6186	48.0676	YES
143	1063.8374	6349.4255	YES
144	1070.9088	95.8992	YES

145	1080.7957	1.6116	YES
146	1084.4561	9.4295	YES
147	1091.7393	2518.3044	YES
148	1094.9135	909.7069	YES
149	1100.6238	39.9075	YES
150	1109.4777	65.9104	YES
151	1113.3997	302.9321	YES
152	1119.2831	1665.3074	YES
153	1124.5091	13.8426	YES
154	1126.6705	434.2178	YES
155	1132.3743	805.9263	YES
156	1149.6831	130.8914	YES
157	1153.5954	86.5840	YES
158	1156.7259	72.3554	YES
159	1168.0476	23.8566	YES
160	1174.4163	50.6980	YES
161	1182.4419	653.9989	YES
162	1184.8474	214.1128	YES
163	1185.4367	4.6781	YES
164	1188.3699	1348.6797	YES
165	1188.5629	79.0795	YES
166	1213.1862	20.9591	YES
167	1216.4994	12.9909	YES
168	1217.1622	94.5560	YES
169	1222.0180	85.7346	YES
170	1228.0097	178.9304	YES
171	1237.5219	398.9908	YES
172	1241.2110	954.4653	YES
173	1254.7579	52.8514	YES
174	1260.3025	50.2181	YES
175	1277.5423	1259.5334	YES
176	1288.1869	135.4177	YES
177	1292.7093	28.3234	YES
178	1300.8816	101.7507	YES
179	1302.3593	77.6566	YES
180	1304.2346	645.7066	YES
181	1308.6153	58.8695	YES
182	1309.9370	864.9925	YES
183	1321.5045	72.4004	YES
184	1327.9081	186.2202	YES
185	1332.0133	100.0313	YES
186	1339.4764	106.8556	YES
187	1341.6200	119.1917	YES
188	1343.9960	7.3324	YES

189	1352.4899	174.5739	YES
190	1360.5770	526.6747	YES
191	1369.1255	147.8325	YES
192	1371.2173	98.6539	YES
193	1371.9257	122.1696	YES
194	1387.0504	265.5215	YES
195	1395.0545	24.1834	YES
196	1396.3004	72.8829	YES
197	1404.1643	195.4407	YES
198	1406.0740	120.2941	YES
199	1410.3337	39.4991	YES
200	1411.7455	77.2280	YES
201	1414.8293	348.9306	YES
202	1414.9137	16.6810	YES
203	1416.1597	22.8420	YES
204	1419.0926	100.1176	YES
205	1419.3477	706.1636	YES
206	1421.6060	564.4224	YES
207	1423.0687	604.5728	YES
208	1424.8953	5.1752	YES
209	1428.5240	121.0935	YES
210	1431.5484	16.5966	YES
211	1436.2335	337.3581	YES
212	1441.2008	42.8564	YES
213	1449.8457	57.7754	YES
214	1451.3997	84.0935	YES
215	1456.5378	73.1850	YES
216	1478.8387	204.6058	YES
217	1485.0908	12.1451	YES
218	1485.7528	3.7813	YES
219	1487.0785	9.7448	YES
220	1488.3281	496.3047	YES
221	1489.4413	35.1117	YES
222	1492.4220	5.6801	YES
223	1493.3654	5.1015	YES
224	1494.4584	11.3638	YES
225	1495.6239	17.8610	YES
226	1497.0880	9.4864	YES
227	1497.4802	34.1812	YES
228	1498.1365	92.7971	YES
229	1498.7456	5.5849	YES
230	1499.7476	137.4870	YES
231	1500.9262	15.5179	YES
232	1501.2985	39.1415	YES

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233	1504.4987	63.1507	YES
234	1504.9110	192.0772	YES
235	1508.7150	113.0818	YES
236	1510.0295	159.0907	YES
237	1510.8247	310.6196	YES
238	1511.9948	42.8844	YES
239	1515.8285	17.4036	YES
240	1516.3972	24.7820	YES
241	1520.1461	50.3387	YES
242	1521.6075	41.6317	YES
243	1538.5048	26.6101	YES
244	1540.2094	148.3388	YES
245	1542.1414	392.7726	YES
246	1542.4840	209.4448	YES
247	1548.2040	388.4519	YES
248	1557.5911	3072.6159	YES
249	1575.8485	227.6789	YES
250	1602.8109	133.7430	YES
251	1628.0524	624.4535	YES
252	1647.4680	87.1272	YES
253	1676.7024	30.5547	YES
254	1678.5109	22.5228	YES
255	1687.8712	9.2618	YES
256	1689.7801	7.0166	YES
257	3034.5002	38.8152	YES
258	3040.5176	50.7495	YES
259	3047.1052	26.3923	YES
260	3053.1531	62.8075	YES
261	3053.7370	43.5471	YES
262	3054.5098	21.9025	YES
263	3055.4614	33.6343	YES
264	3055.9470	31.3038	YES
265	3058.6034	86.2431	YES
266	3060.0538	36.1754	YES
267	3060.7596	32.2317	YES
268	3064.4534	37.1487	YES
269	3066.0686	26.0032	YES
270	3068.0531	25.2911	YES
271	3070.2785	32.3263	YES
272	3072.5256	79.1587	YES
273	3101.1511	66.7624	YES
274	3103.1458	32.2865	YES
275	3106.5459	106.4271	YES
276	3107.9722	61.2636	YES

277	3109.5949	31.3900	YES
278	3123.8464	26.5145	YES
279	3126.5074	19.3065	YES
280	3127.1604	31.8383	YES
281	3128.4555	32.8839	YES
282	3131.1842	19.3438	YES
283	3131.5432	81.2077	YES
284	3132.7817	30.3000	YES
285	3133.8023	62.0520	YES
286	3137.5808	45.9866	YES
287	3137.8385	20.5830	YES
288	3137.8888	62.0011	YES
289	3139.9864	50.7282	YES
290	3140.1524	58.0256	YES
291	3142.6580	49.2437	YES
292	3145.3461	48.3912	YES
293	3147.8036	49.8602	YES
294	3151.7077	42.4899	YES
295	3152.9213	42.5718	YES
296	3157.6337	46.3952	YES
297	3158.0135	43.3141	YES
298	3158.3880	37.0233	YES
299	3162.9354	33.9124	YES
300	3178.5534	59.6108	YES
301	3180.1196	36.9241	YES
302	3192.8261	4.4327	YES
303	3194.9847	1.4176	YES
304	3201.6777	11.1148	YES
305	3203.9393	16.2191	YES
306	3215.0516	28.1069	YES
307	3216.2461	44.9216	YES
308	3219.5993	18.6391	YES
309	3223.4524	34.6409	YES
310	3225.8171	11.5403	YES
311	3228.5425	21.4599	YES
312	3246.1456	10.5875	YES
313	3257.4116	7.7340	YES
314	3616.3670	22.8075	YES
315	3731.1068	10.2583	YES

Cy-Oam

mode	wave number cm^{-1}	IR intensity km/mol	selection rules IR
1	14.8623	1.2652	YES

2	17.7122	0.4225	YES
3	21.8882	0.9000	YES
4	29.2484	1.7554	YES
5	33.1318	0.1297	YES
6	37.5550	0.2212	YES
7	46.1314	5.4224	YES
8	51.7163	1.4589	YES
9	60.5174	6.7951	YES
10	69.6340	0.1927	YES
11	71.7349	5.1175	YES
12	76.2721	0.3673	YES
13	83.3797	1.0653	YES
14	83.7046	10.6116	YES
15	91.5957	3.9755	YES
16	95.4749	3.8598	YES
17	110.6119	4.2069	YES
18	116.5312	3.6266	YES
19	129.6435	2.0294	YES
20	139.5193	11.0324	YES
21	142.6918	22.2323	YES
22	143.7970	8.1318	YES
23	152.3123	64.2010	YES
24	160.1285	8.0639	YES
25	182.4422	53.8215	YES
26	190.3264	9.1990	YES
27	198.7886	68.0331	YES
28	204.4947	4.2258	YES
29	214.9120	0.2313	YES
30	223.3527	12.6237	YES
31	227.5018	6.3653	YES
32	238.6299	9.0061	YES
33	241.4011	0.9906	YES
34	242.1412	9.2738	YES
35	250.3875	9.8094	YES
36	253.2449	6.0607	YES
37	261.2489	32.3771	YES
38	264.9071	5.3559	YES
39	266.9987	49.6529	YES
40	275.0347	1.5931	YES
41	279.8872	0.5035	YES
42	283.0365	24.7623	YES
43	287.4262	2.2290	YES
44	294.4627	2.1123	YES
45	296.5089	1.1875	YES

46	299.7535	23.4120	YES
47	308.7894	5.0715	YES
48	311.3879	210.4541	YES
49	315.8254	194.7589	YES
50	321.3521	189.0868	YES
51	334.2685	11.4170	YES
52	344.8354	17.5003	YES
53	353.3665	61.0532	YES
54	358.2222	6.2304	YES
55	360.2887	1.4511	YES
56	364.0164	8.8088	YES
57	367.1861	10.9684	YES
58	375.2216	98.0515	YES
59	406.7565	31.6996	YES
60	417.7374	93.6588	YES
61	418.2655	36.5842	YES
62	424.8518	18.6638	YES
63	433.2678	155.8434	YES
64	439.7778	10.4656	YES
65	446.4204	116.9204	YES
66	463.5248	14.6485	YES
67	476.0439	35.5641	YES
68	482.8366	34.9518	YES
69	489.5404	105.1013	YES
70	490.2926	9.8812	YES
71	493.3389	24.0441	YES
72	504.0872	68.7934	YES
73	510.1087	6.4900	YES
74	537.4318	734.5098	YES
75	553.4900	1301.8664	YES
76	565.1661	76.2240	YES
77	568.1122	14.6608	YES
78	569.2617	117.4897	YES
79	577.7294	316.1969	YES
80	582.2135	6.7397	YES
81	585.2190	9.5809	YES
82	594.6093	14.8520	YES
83	596.3569	5.2372	YES
84	630.6264	0.1126	YES
85	633.3623	8.2032	YES
86	645.6668	1171.6524	YES
87	665.3788	13.4832	YES
88	690.4506	246.1023	YES
89	709.6327	49.3223	YES

90	715.2868	4.4236	YES
91	718.6720	395.8344	YES
92	729.1902	2537.5234	YES
93	748.3097	911.5760	YES
94	758.7615	133.0049	YES
95	762.8569	626.9713	YES
96	764.0922	91.7880	YES
97	765.9429	1462.8559	YES
98	773.6085	146.2573	YES
99	785.4849	48.4379	YES
100	786.8697	10.7133	YES
101	791.1282	2285.6626	YES
102	798.4054	34.4165	YES
103	825.7075	1825.6659	YES
104	830.8327	5.0995	YES
105	837.3842	205.0251	YES
106	849.6107	336.7226	YES
107	854.9819	762.6635	YES
108	859.1650	175.1089	YES
109	867.0377	546.8326	YES
110	869.6604	232.5907	YES
111	885.3785	361.9233	YES
112	886.3680	3754.0375	YES
113	889.8171	1.6784	YES
114	893.0914	59.8471	YES
115	912.0453	901.8586	YES
116	924.6891	2340.2884	YES
117	934.5314	9184.9833	YES
118	935.3953	2049.3364	YES
119	945.5045	1278.4429	YES
120	954.5642	442.1709	YES
121	958.3556	2618.5760	YES
122	966.4843	90.9021	YES
123	968.0554	288.0566	YES
124	969.1454	21.9625	YES
125	970.3854	6.7913	YES
126	972.7177	378.9601	YES
127	974.3958	51.3059	YES
128	977.6509	126.6367	YES
129	978.9983	98.2850	YES
130	987.5931	1850.8697	YES
131	990.3955	484.4958	YES
132	992.7831	283.8577	YES
133	1006.6440	0.1540	YES

134	1017.0209	1.5565	YES
135	1017.9561	132.7880	YES
136	1029.7947	19440.5212	YES
137	1045.6158	444.0427	YES
138	1055.0838	140.2825	YES
139	1056.7896	313.5793	YES
140	1058.7973	121.8456	YES
141	1060.5747	285.8462	YES
142	1063.8860	2593.5880	YES
143	1072.5614	20.9231	YES
144	1085.1412	24.9215	YES
145	1086.8347	0.5514	YES
146	1091.8977	2389.9849	YES
147	1098.7627	33.0190	YES
148	1113.4201	35.9908	YES
149	1115.0018	78.2098	YES
150	1122.8749	920.9241	YES
151	1129.0635	212.4076	YES
152	1129.3090	29.3123	YES
153	1130.1329	1052.5117	YES
154	1144.6918	12.2481	YES
155	1150.9052	124.9697	YES
156	1156.1505	60.1321	YES
157	1166.5231	33.4290	YES
158	1176.1044	34.0980	YES
159	1181.7751	1155.3286	YES
160	1185.3230	90.8531	YES
161	1185.8278	13.6973	YES
162	1186.1823	80.1108	YES
163	1186.9172	55.0768	YES
164	1189.9528	947.8811	YES
165	1205.6698	41.4484	YES
166	1214.5687	34.0557	YES
167	1217.4763	15.4993	YES
168	1222.8542	35.7695	YES
169	1240.8546	1143.7889	YES
170	1244.8075	313.7230	YES
171	1256.7236	115.8630	YES
172	1258.6143	30.9886	YES
173	1276.0818	80.3463	YES
174	1278.5460	1502.4113	YES
175	1286.0343	59.0849	YES
176	1299.1844	181.3430	YES
177	1302.5634	264.0653	YES

178	1304.5665	64.5726	YES
179	1306.0435	102.7710	YES
180	1311.2224	704.2693	YES
181	1321.9531	64.2952	YES
182	1327.8737	174.3134	YES
183	1335.0688	100.2057	YES
184	1338.4104	28.4999	YES
185	1345.0400	35.7076	YES
186	1346.1289	10.8005	YES
187	1352.0446	234.9440	YES
188	1360.3313	438.0562	YES
189	1369.1697	169.1136	YES
190	1375.7543	25.8758	YES
191	1377.1530	58.0097	YES
192	1390.9469	3.0556	YES
193	1393.0516	197.1492	YES
194	1402.0312	109.6076	YES
195	1405.2913	269.7209	YES
196	1415.2702	267.9910	YES
197	1417.1539	225.4273	YES
198	1418.2753	1477.5244	YES
199	1419.9989	7.8984	YES
200	1421.6374	120.3376	YES
201	1423.2904	106.6648	YES
202	1425.2459	13.9332	YES
203	1427.1502	14.1612	YES
204	1428.6240	11.7332	YES
205	1430.5321	12.3600	YES
206	1431.7825	13.8783	YES
207	1436.0873	15.2277	YES
208	1439.6199	343.4394	YES
209	1444.5903	260.4608	YES
210	1456.4153	165.4897	YES
211	1457.5383	36.2829	YES
212	1458.3305	66.2242	YES
213	1476.0377	288.8679	YES
214	1482.1723	1.7708	YES
215	1485.2161	15.4921	YES
216	1487.7093	259.7158	YES
217	1488.3326	184.2591	YES
218	1490.8647	16.6617	YES
219	1491.5399	38.8736	YES
220	1492.0563	4.1078	YES
221	1496.0875	3.1238	YES

222	1497.0787	12.0667	YES
223	1497.5470	17.1982	YES
224	1497.9038	30.3221	YES
225	1498.5898	56.6440	YES
226	1499.8939	108.8921	YES
227	1500.7722	20.3406	YES
228	1500.8202	3.3357	YES
229	1502.4264	165.0262	YES
230	1503.7668	13.7511	YES
231	1504.6510	9.4565	YES
232	1507.4046	176.1605	YES
233	1508.4569	47.7022	YES
234	1509.0428	100.9464	YES
235	1510.7980	252.9498	YES
236	1512.0840	12.4652	YES
237	1516.1749	6.6817	YES
238	1519.1119	58.9742	YES
239	1523.3989	8.5811	YES
240	1525.2412	12.6937	YES
241	1531.2422	138.9981	YES
242	1535.4207	114.5083	YES
243	1542.8915	267.4896	YES
244	1543.1044	119.1166	YES
245	1564.4998	3292.6303	YES
246	1573.0150	81.2172	YES
247	1599.8657	105.5381	YES
248	1630.1409	542.0862	YES
249	1646.6857	174.1824	YES
250	1676.4233	22.2269	YES
251	1676.5775	27.6547	YES
252	1688.2307	8.0594	YES
253	1689.4365	9.9046	YES
254	1790.2983	179.3436	YES
255	3031.8446	40.1440	YES
256	3042.2860	47.4297	YES
257	3054.4832	47.4290	YES
258	3056.6055	33.3793	YES
259	3060.2702	36.1346	YES
260	3061.2539	30.5116	YES
261	3062.6880	43.1566	YES
262	3065.1617	20.4675	YES
263	3066.2292	13.7714	YES
264	3066.9529	30.0783	YES
265	3071.2790	16.1929	YES

266	3073.2633	77.9112	YES
267	3075.8533	12.7808	YES
268	3076.7107	16.0630	YES
269	3079.9071	5.1802	YES
270	3085.7155	8.6247	YES
271	3103.3557	69.2495	YES
272	3106.1783	64.8364	YES
273	3108.0179	100.6987	YES
274	3124.3357	8.5695	YES
275	3129.3435	15.5670	YES
276	3133.9422	15.5280	YES
277	3136.7331	26.3543	YES
278	3137.0706	20.3848	YES
279	3137.8365	6.4458	YES
280	3138.8326	55.1250	YES
281	3139.1147	42.6518	YES
282	3139.2469	41.8745	YES
283	3139.8214	47.0752	YES
284	3143.7629	52.7798	YES
285	3152.6872	43.7549	YES
286	3154.6951	47.0530	YES
287	3157.3581	47.0424	YES
288	3159.3279	6.9091	YES
289	3160.6517	46.3865	YES
290	3162.0394	5.1803	YES
291	3162.5090	14.6014	YES
292	3164.1103	40.6601	YES
293	3165.4129	5.3246	YES
294	3167.8454	11.4842	YES
295	3170.0507	19.7211	YES
296	3171.7541	20.3420	YES
297	3185.1109	35.2936	YES
298	3189.0262	10.0217	YES
299	3192.9580	4.0667	YES
300	3193.6092	0.5779	YES
301	3202.5154	10.9940	YES
302	3203.5644	28.5168	YES
303	3205.9323	14.8238	YES
304	3215.0448	31.8669	YES
305	3215.0675	47.9507	YES
306	3224.1455	35.7915	YES
307	3225.1715	3.5298	YES
308	3231.6118	26.1027	YES
309	3232.0252	16.5264	YES

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310	3237.1266	18.3490	YES
311	3267.9514	8.1605	YES
312	3600.2741	27.4564	YES