Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Not in black or white, encryption of grayscale images by donor-acceptor Stenhouse adducts

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Contents

1. Experimental section

1.1. Material

All the chemicals and reagents were commercially obtained and used without further purification. 2-furaldehyde ($C_5H_4O_2$, CAS No. 98-01-1), N-propylaniline ($C_9H_{13}N$, CAS No. 622-80-0), Glycerol triacetate (GTA) ($C_9H_{14}O_6$, CAS No. 102-76-1), was purchased from the Aladdin Chemicals. Hexyl benzoate (HB) ($C_{13}H_{18}O_2$, CAS No. 6789-88-4), Hexyl hexanoate (HH) ($C_{12}H_{24}O_2$, CAS No. 6378-65-0), Triethylene glycol diacetate (TGD)($C_{10}H_{18}O_6$, CAS No. 111-21-7), Polymethyl methacrylate (PMMA) ($(C_5H_8O_2)n$, M_n=800000 g/mol, CAS No. 9011-14-7), were purchased from Macklin. Ethanol (C_2H_6O, CAS No. 64-17-5) Tetrahydrofuran (THF)(C_4H_8O, CAS No. 109-99-9),

Acetonitrile (C_2H_3N, CAS No. 75-05-8) and methylene dichloride (DCM) (CH_2Cl_2, CAS No. 75-09-2) were purchased from Chengdu Keshi Reagent. Milli-Q water (resistivity: 18.2 MΩ×cm) was used throughout the project.

1.2. Characterizations methods

UV-vis spectra (including absorbance and reflectance) were recorded on a Shimazu UV-2600 spectrophotometer. For the determination of the kinetics of isomerization between *linear* and *cyclic* donor-acceptor Stenhouse adducts (DASAs), the absorbance (reflectance) value at a typical wavelength was recorded to obtain precise results. The content of *cyclic* isomers was calculated as described in **section 3**.

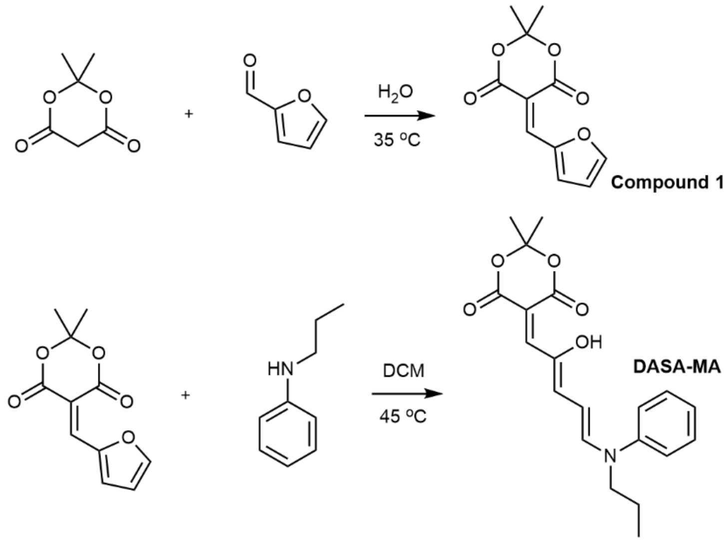
Density functional theory (DFT) calculation was used to understand the relative pKa and molecular energy variation during the isomerization between *linear* and *cyclic* DASAs. Moreover, the length of the intramolecular hydrogen bond was calculated under surrounding functional molecules. These were described in detail in **section 4**.

For the controlling of isomerization between *linear* and *cyclic* DASAs, light-emitting diodes (LED) systems generating 520 nm green light was used to induce the *linear*-to-*cyclic* isomerization of DASAs in solutions, on paper surfaces (Zhongjiao Jinyuan Systems). The output intensity of the

LED was controlled by an LED controller (Zhongjiao Jinyuan Systems) and calibrated by a Laserpoint calibrator (A-02-D12-BBF). A uniformly exposed LED white light (10,000) was used for recording videos in Fig. 3 and Supplementary videos 1-4.

For the printing of ester-contained invisible inks dissolved in EtOH, a commercial ink-jet printer (EPSON L130) was used.

1.3. Synthesis of DASA-MA



Scheme S1. Synthetic route for **DASA-MA**

*Synthesis of **DASA-MA.*** Synthesis of DASAs is according to previous reports without modifications.[1, 2] 2,2-dimethyl-1,3-dioxane-4,6-dione (1 g, 6.93 mmol) was completely dissolved into 20 mL distilled water under stirring. 2-furaldehyde (666.62 mg, 6.93 mmol) was slowly dropped into the solution. Then, the solution was heated to 35 °C and kept for 2 h, which formed a yellow solid. The yellow solid was collected by vacuum filtration, followed by washing with distilled water for several times. The solid was then dissolved into 50 mL methylene dichloride and washed by 50 mL saturated NaCl aqueous solution. The organic layer was purified by column chromatography, and obtained a yellow solution which was then condensed by rotary evaporation to give 1.233 g yellow product (Yield: 95 %). The yellow product (300 mg, 1.35 mmol) was dissolved into 20 mL DCM, followed by slowly adding N-Propylaniline (182 mg, 1.35 mmol) under stirring. After stirring at 40 °C for 2 h, the solution turned to deep purple. The mixture was then condensed by rotary evaporation and further purified by column chromatography to give 289 mg (Yield: 60 %) deep purple solid **DASA-MA**. Crystal structure data for **DASA-MA** can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif CCDC# 2258697

2. Photoisomerization of DASAs in solvents

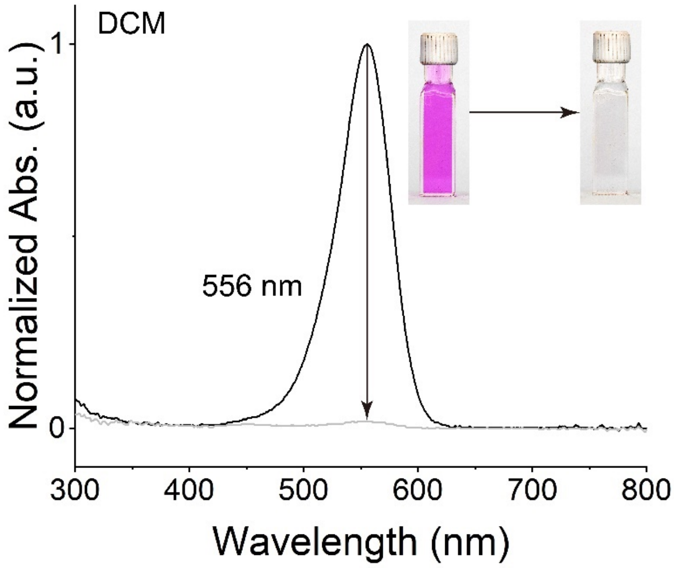


Fig. S1. Normalized UV-Vis absorption spectra of **DASA-MA** before and after green light irradiation (520 nm, 40 mW/cm^2, 1 min) in DCM. Inner shows the photographic images before and after green light irradiation.

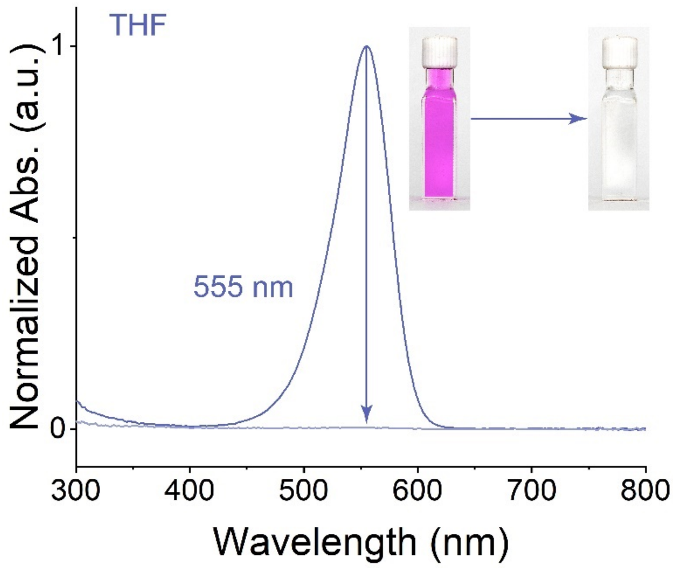


Fig. S2. Normalized UV-Vis absorption spectra of **DASA-MA** before and after green light irradiation (520 nm, 40 mW/cm^2, 1 min) in THF. Inner shows the photographic images before and after green light irradiation.

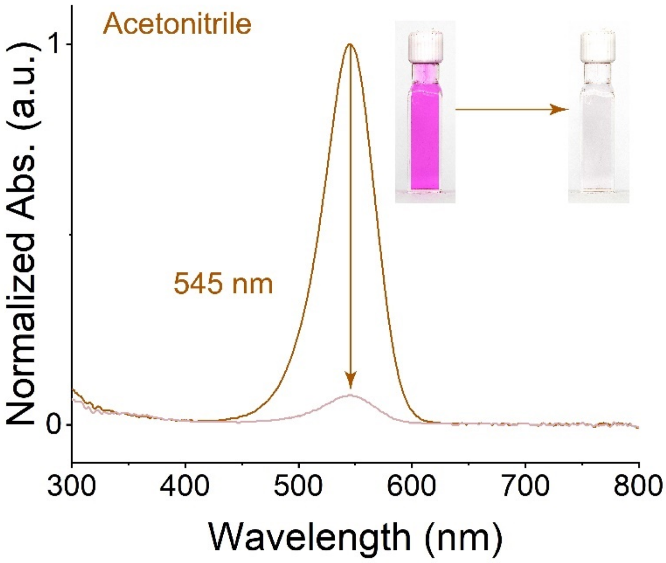


Fig. S3. Normalized UV-Vis absorption spectra of **DASA-MA** before and after green light irradiation (520 nm, 40 mW/cm^2, 1 min) in acetonitrile. Inner shows the photographic images before and after green light irradiation.

3. Photoisomerization of DASAs on the paper surfaces

The isomerization of **DASA-MA** on the paper surfaces under the promotion of ester-contained molecules was investigated by impregnation treatment. For example, to investigate the promotion by **GTA**, four 100 mL portions of 1 mg/mL **DASA-MA**/DCM solution were prepared, the amount of **DASA-MA** in each portion of the solution was 100 mg, followed by adding 0 mg, 100 mg, 200 mg, and 500 mg of **GTA** sequentially to the solution, and followed by impregnating the papers to the above solution for 30 s and dried in the dark at room temperature for 3 min. The samples were named 0, 1, 2 and 5, respectively, based on the mass ratio of **GTA**:**DASA-MA**.

Due to each scanning process taking 85 s, the real-time counting method was used to capture the peak reflectance, to get the reflectance at a specific time (R_t), DASAs in *cyclic* do not absorb in the visible light region,[3-6] therefore, the *linear*-to-*cyclic* isomerization induces the increase in reflectance. Therefore, the portion of *cyclic* DASAs at any given time (C_t) was obtained by the following equation.

$$C_t = \frac{R_{0\,s} - R_t}{R_{Paper-}R_{0\,s}} \times 100\% \quad (1)$$

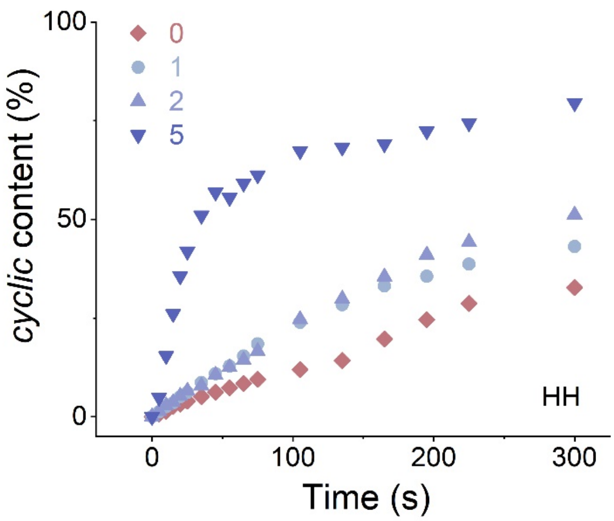


Fig. S4. Time-dependent *linear*-to-*cyclic* (520 nm, 40 mW/cm^2) isomerization of **DASA-MA** on the paper surface using **HH** as the additives (**HH**/**DASA-MA** = 0-5 in weight ratio).

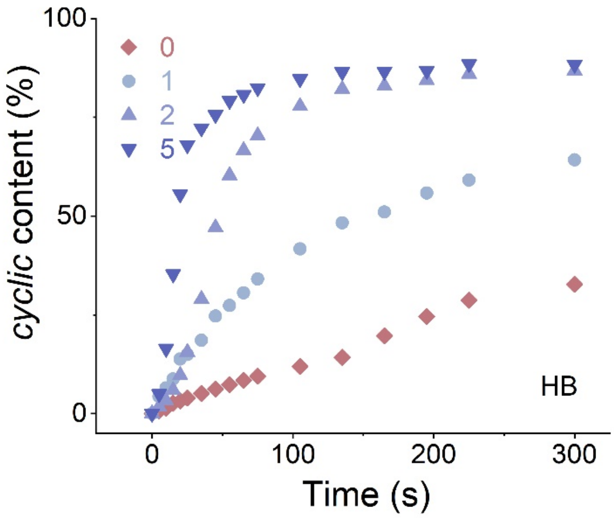


Fig. S5. Time-dependent *linear*-to-*cyclic* (520 nm, 40 mW/cm^2) isomerization of **DASA-MA** on the paper surface using **HB** as the additives (**HB**/**DASA-MA** = 0-5 in weight ratio).

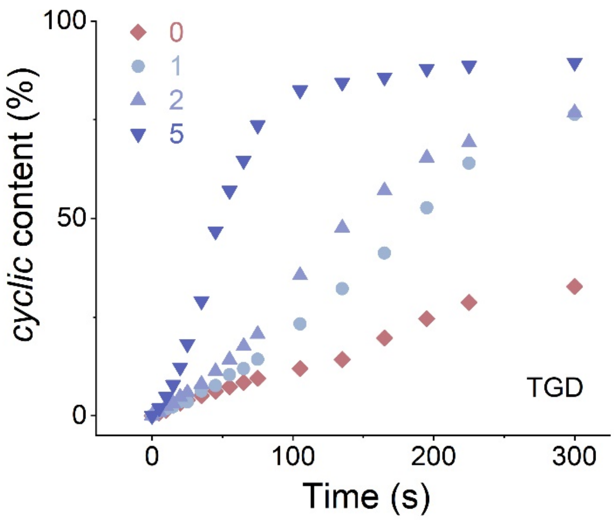


Fig. S6. Time-dependent *linear*-to-*cyclic* (520 nm, 40 mW/cm^2) isomerization of **DASA-MA** on the paper surface using **TDG** as the additives (**TDG**/**DASA-MA** = 0-5 in weight ratio).

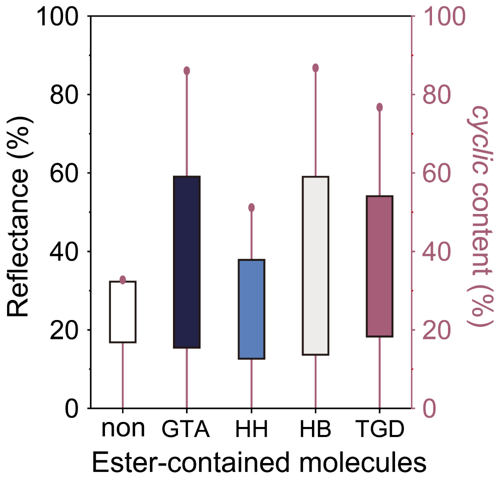


Fig. S7. Summarization of reflectance changes (left, %) and *cyclic* content (right, %) of **DASA-MA** with or without the promotion of 2 mg/mg (**Ester-contained molecules**/**DASA-MA**) under 40 mW/cm^2 520 nm irradiation for 300 s.

4. DFT calculations

Geometry optimizations were performed with the Gaussian 16 program suite[7] using the density functional theory (DFT) with the B3LYP(D3) exchange-correlational functionals[8] and employing the TZVP basis setfor all atoms.[9, 10] The obtained stationary points were characterized by frequency calculations. The calculated geometries were shown in **section 14**.

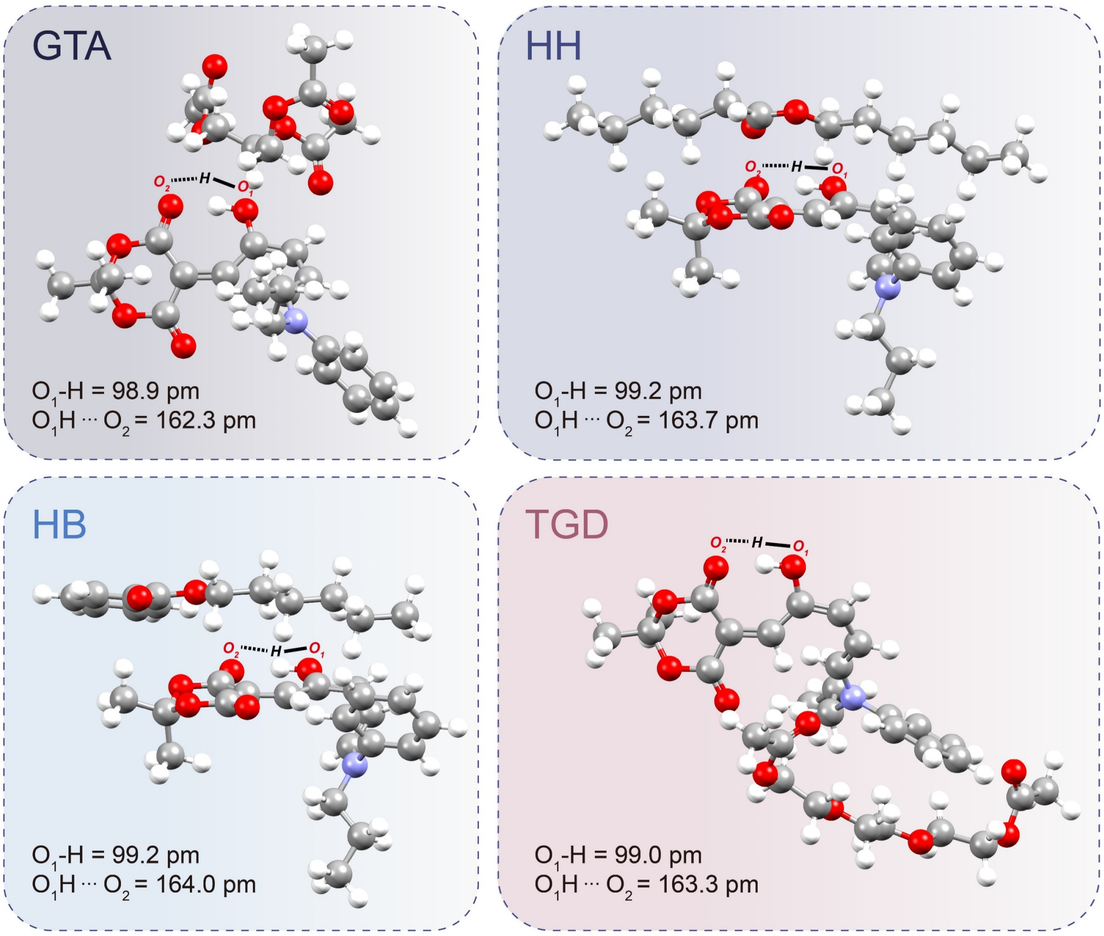


Fig. S8. Schematic illustration of the calculated molecular structure of **DASA-MA** in the A`` state surrounded by **GTA**, **HH**, **HB** and **TGD**.

5. Interrelationship between DFT calculations and isomerization kinetics

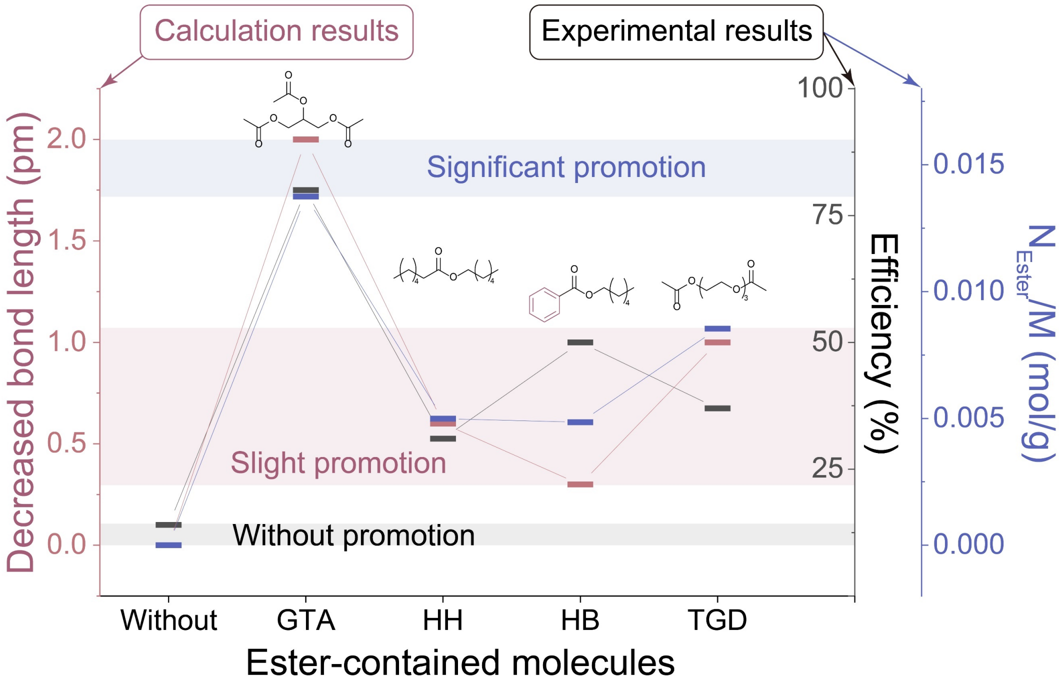


Fig. S9. Calculated decreased length of the intramolecular hydrogen bond of **DASA-MA** with various esters (left red axis); the *linear*-to-*cyclic* isomerization efficiency of **DASA-MA** with various esters (1:1 in weight ratio) after irradiation at 520 nm (40 mW/cm²) for 150 s (right black axis); calculated N_{Ester}/M of various esters (right blue axis).

Five main intermediates are involved during the *linear*-to-*cyclic* photoisomerization of **DASA-MA** (**Fig. 2a**). The intramolecular proton transfer from the hydroxyl group on the triene π-bridge to the carbonyl group on the electron-withdrawing moiety is critically important for the cyclization[1]. Therefore, the length of the intramolecular hydrogen bond closely affects the proton transfer.

The calculated intramolecular hydrogen bond length follows the order of **GTA** < **TGD** < **HH** < **HB**, which was inferred based on well-established principles and assumptions. However, the theoretical predictions are based on simplified models and may not capture all the complexities of real-world systems. A more in-depth analysis was conducted based on the contents of ester groups of the additives with the same weight.

Adding esters obviously decreases the hydrogen bond length as well as promoting the photoisomerization (Fig. S9). The promoting effect could be categorized into three stages: (1) In the absence of additives (bond length of ~164.3 pm), only ~14% *linear* **DASA-MA** isomerize to *cyclic* after 520 nm green light irradiation (40 mW/cm^2) for 150 s (grey region in Fig. S9); (2) Adding **GTA** decreases the hydrogen bond length by 2 pm, and the *linear*-to-*cyclic* transition efficiency sharply reaches ~80% (blue region in Fig. S9); (3) The other additives (**TGD**, **HH** and **HB**) decreased the hydrogen bond length by 0.3-1 pm promote the *linear*-to-*cyclic* transition efficiency to 30-50% (red region in Fig. S9). Therefore, the promoting effect of the photoisomerization exhibits semi-quantitative interrelationship with the decreased value of hydrogen bond length.

In the experiments, the amount of ester-containing additives was determined based on the mass ratio. However, it's important to note that each additive contains a varying number of ester groups as well as a distinct relative molecular mass. To further quantitatively investigate the relationship between experimental and simulation results, the N_{Ester}/M (the amount of the ester groups divided by corresponding molecular weight) was considered, indicating the molar quantity of ester groups on the additives with equal weight (Equation S1).

$$\frac{N_{Ester}}{M} = \frac{m}{M} \times N_{Ester} \qquad S1$$

where N_{Ester} indicates the number of ester groups on each molecule; M represents the molecular weight; m represents the mass of the additives.

GTA with 3 ester groups shows the highest value of N_{Ester}/M (~0.013), indicating the strongest contribution of esters (blue line in Fig. S9). On the contrary, **TGD**, **HB** and **HH** with 1 or 2 ester groups exhibit lower values of N_{Ester}/M. These are in good accordance with the results of promoting effect of photoisomerization of **DASA-MA**. Therefore, both the length of intramolecular hydrogen bond and the content of ester groups affect the *linear*-to-*cyclic* isomerization of **DASA-MA**.

6. Solvatochromism of DASA-MA

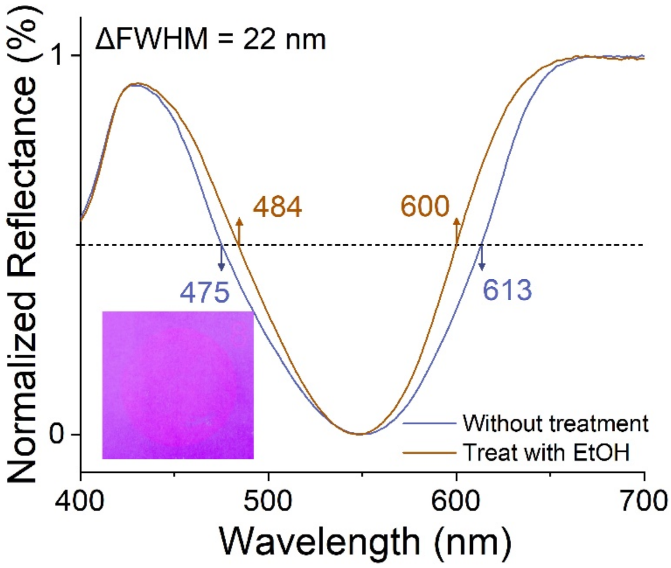


Fig. S10. Normalized reflectance spectra of paper after impregnation in 1 mg/mL **DASA-MA**/DCM solution (blue) and printed with 300 mg/mL **GTA**/EtOH ink (red). Inner show the images of the area with (inner circle) and without (outside the circle) **GTA**/EtOH ink,

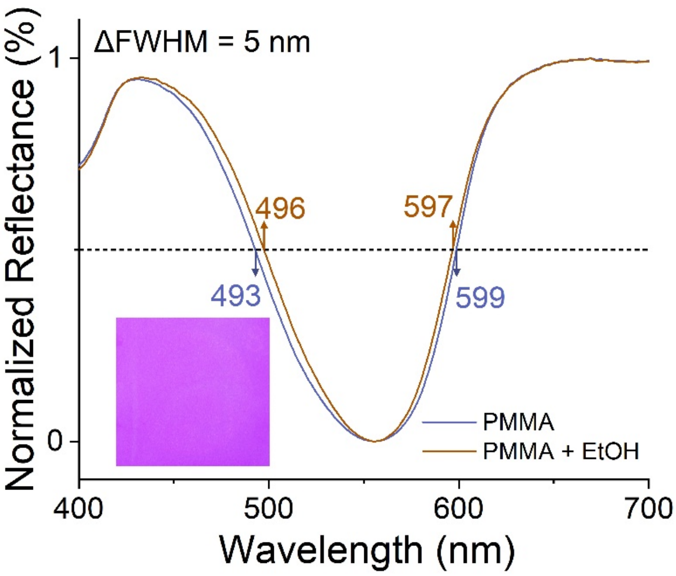


Fig. S11. Normalized reflectance spectra of paper after impregnation in 1 mg/20 mg/mL **DASA-MA**/PMMA/DCM solution (blue) and printed with 300 mg/mL **GTA**/EtOH ink (red). Inner show the images of the area with (inner circle) and without (outside the circle) **GTA**/EtOH ink.

The boiling point of **GTA** is 258-260 °C. Therefore, **GTA** is deposited on paper surface after printing, which promotes the *linear*-to-*cyclic* isomerization of **DASA-MA**. The reflectance spectra of **DASA-MA** on paper surface with and without the addition of **GTA** (1 mg/mL) were compared (Fig. S12). The addition of **GTA** does not lead to any significant changes in the reflectance spectra. Nevertheless, upon the addition of PMMA, there is an increase of reflectance between 200-300 nm, and a notable reduction of the full width at half maximum (FWHM) of the reflectance in visible light region. Therefore, the intermolecular interaction between **GTA** and **DASA-MA** might be too weak to be recognized by reflectance spectra.

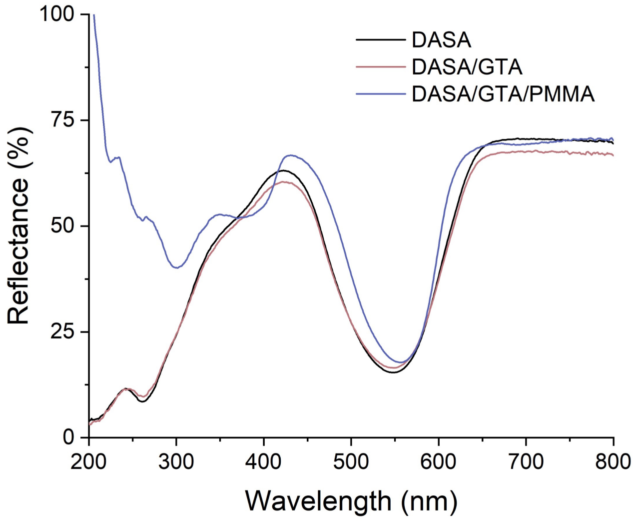


Fig. S12. Reflectance spectra of paper treated with **DASA-MA**/DCM = 1 mg/1 mL(black), **DASA-MA**/**GTA**/DCM = 1 mg/1 mg/1 mL (red) and **DASA-MA**/**GTA**/**PMMA** = 1 mg/1 mg/20 mg/1 mL (blue) solutions.

The chemistry on paper surface was monitored by ATR-FTIR spectroscopy. After immersing the paper in a 1 mg/mL **DASA-MA** solution, there were no significant changes between ~1600-1000 cm^{-1}. Peaks attributed to the vibration of benzene rings and double bonds on the triene π-bridge of **DASA-MA** are observed in the fingerprint region at ~825-710 cm^{-1} (Fig. S13). After introducing **GTA**, a broad peak at ~1647 cm^{-1} emerges due to the vibration of C=O of ester groups (Fig. S13).

Finally, with the introduction of **PMMA**, a distinct peak at ~1733 cm^{-1} appears due to the vibration of C=O (Fig. S13). Due to the weak signals of ATR-FTIR spectra, it is difficult to recognize the intermolecular interaction between the molecules.

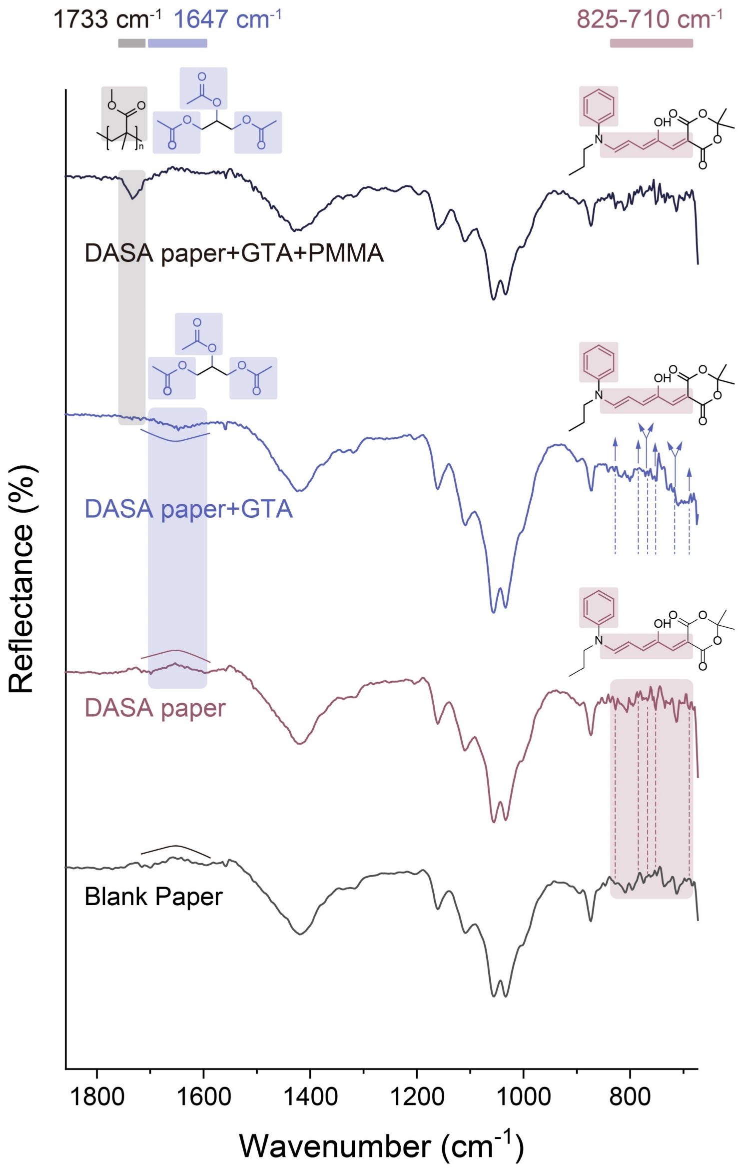


Fig. S13. ATR-FTIR spectra of pure paper (black), paper treated with **DASA-MA**/DCM = 1 mg/1 mL (red), **DASA-MA**/**GTA**/DCM = 1 mg/1 mg/1 mL (blue) and **DASA-MA**/**GTA**/PMMA = 1 mg/1 mg/20 mg/1 mL (gray) solutions.

7. Photoisomerization of DASA-MA on the PMMA pretreated paper surfaces

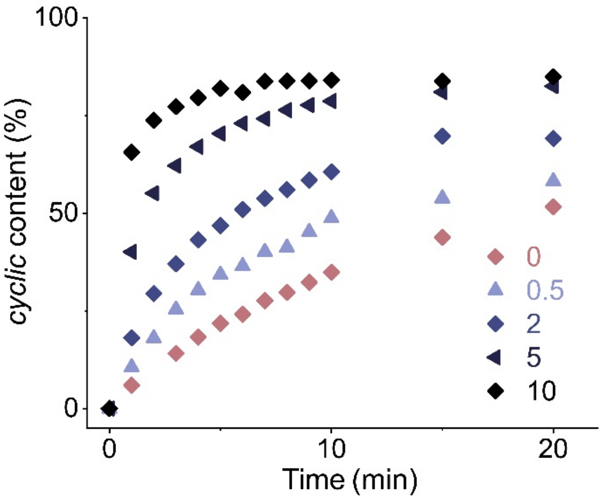


Fig. S14. Time-dependent *linear*-to-*cyclic* (520 nm, 40 mW/cm^2) isomerization of **DASA-MA** on PMMA pretreated paper surfaces using **GTA** as the additives (**GTA/DASA-MA** = 0-10 in weight ratio).

8. Image processing for grayscale printing

First, the specified image (**Fig. S16**) is converted from an RGB image to a gray image in MATLAB using the following code,

```
rgbImage = imread('image.jpg');
grayImage = rgb2gray(rgbImage);
imshow(grayImage);
```

The above image was then converted grayscale image to 1, 2, 4 bit representation (**Scheme 1a**) in MATLAB through code,

```
gray_img(gray_img <= 127) = 0;
gray_img(gray_img > 127) = 255;
imshow(gray_img);
imwrite(gray_img,' 1bit.jpg', jpg');
gray_img(gray_img <= 42) = 0;
gray_img(gray_img > 42 & gray_img <= 127) = 85;
gray_img(gray_img > 128 & gray_img <= 213) = 170;
gray_img(gray_img > 213) = 255;
imshow(gray_img);
imwrite(gray_img,' . 2bit.jpg ',' jpg ');

ray_img(gray_img <= 7) = 0;
gray_img(gray_img >= 7 & gray_img <= 23) = 15;
gray_img(gray_img > 23 & gray_img <= 39) = 31;
gray_img(gray_img >= 39 & gray_img <= 55) = 47;
gray_img(gray_img > 55 & gray_img <= 71) = 63;
gray_img(gray_img >= 71 & gray_img <= 87) = 79;
gray_img(gray_img > 87 & gray_img <= 103) = 95;
gray_img(gray_img > 103 & gray_img <= 119) = 111;
gray_img(gray_img > 119 & gray_img <= 135) = 127;
gray_img(gray_img > 135 & gray_img <= 151) = 143;
gray_img(gray_img > 151 & gray_img <= 167) = 159;
gray_img(gray_img > 167 & gray_img <= 183) = 175;
gray_img(gray_img > 183 & gray_img <= 199) = 191;
```

```
gray_img(gray_img > 199 & gray_img <= 215) = 207;
gray_img(gray_img > 215 & gray_img <= 231) = 223;
gray_img(gray_img > 231 & gray_img <= 247) = 239;
gray_img(gray_img > 247) = 255;
imshow(gray_img);
imwrite(gray_img,' 4bit.jpg','jpg');
```

Before printing, the above mentioned 1-8 bit images need to go through the reverse processing as below (**Fig. S22**),

```
grayImage = imread('grayscale_image.jpg');
invertedImage = 255 - grayImage;
imshow(invertedImage);
imwrite(invertedImage, 'inverted_image.jpg');
```

The code to output the histogram of the gray scale distribution (**Fig. 3c-e**, **Fig. S24b** and **S17-S21**) is as follows,

```
clear;clc;
  [FileName,FilePath]=uigetfile('*.jpg;*.png;*.tif;*.img;*.gif;');
str=[FilePath,FileName];
color_image=imread(str);
grayscale_image=rgb2gray(color_image);
imshow(grayscale_image);title('Original Grayscale Image');
histogram = imhist(grayscale_image);
figure;
bar(histogram);
title('Grayscale Histogram');
xlabel('Pixel Intensity');
ylabel('Frequency')
```

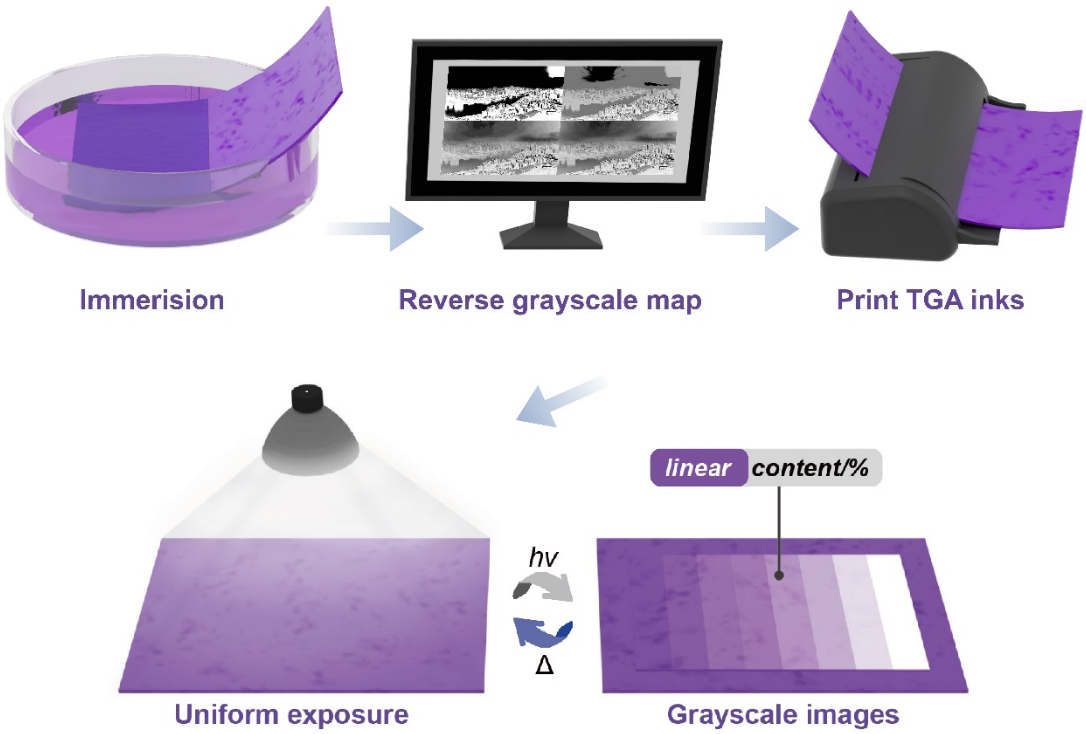


Fig. S15. The schematic illustration of grayscale printing.

Fig. S16. Photographic image of Jialing River (shot by Wang in Chongqing).

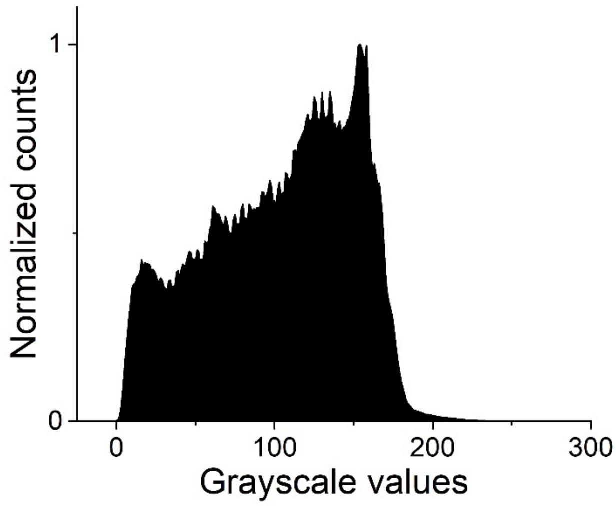


Fig. S17. Normalized brightness distributions of the raw image.

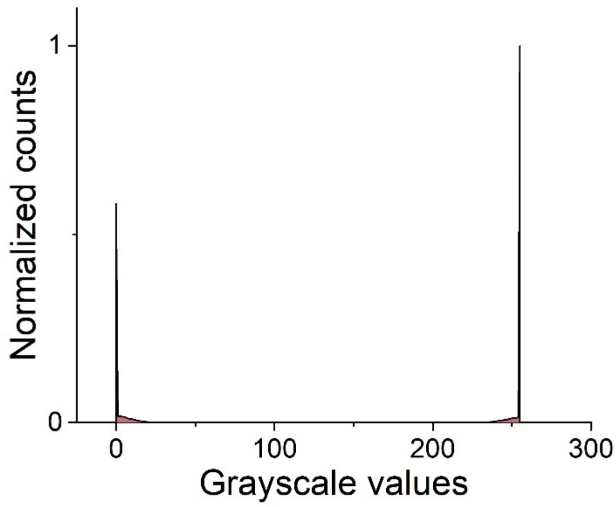


Fig. S18. Normalized brightness distributions of the 1-bit image.

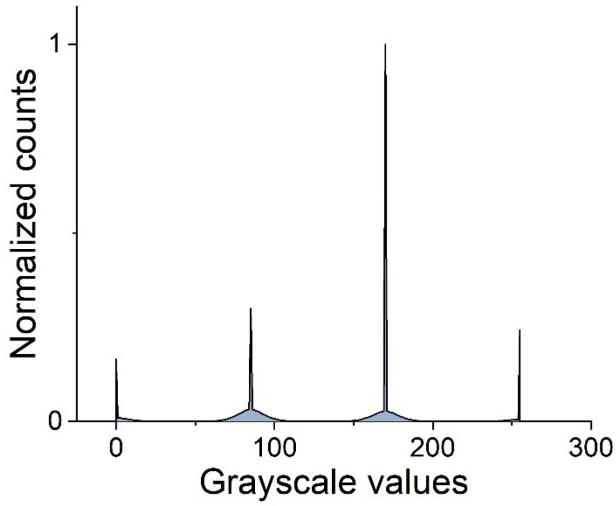


Fig. S19. Normalized brightness distributions of the 2-bit image.

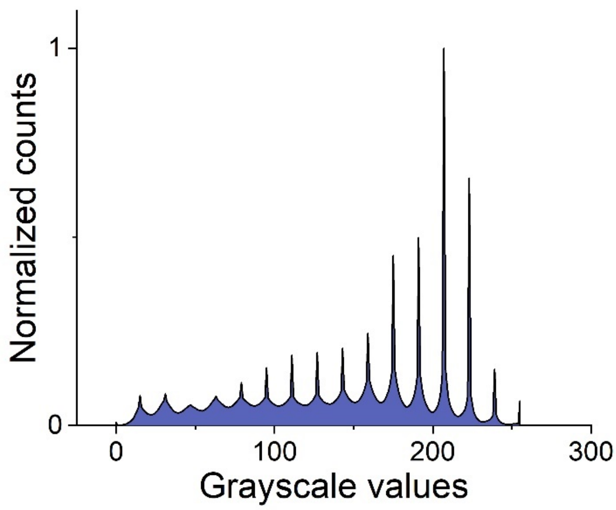


Fig. S20. Normalized brightness distributions of the 4-bit image.

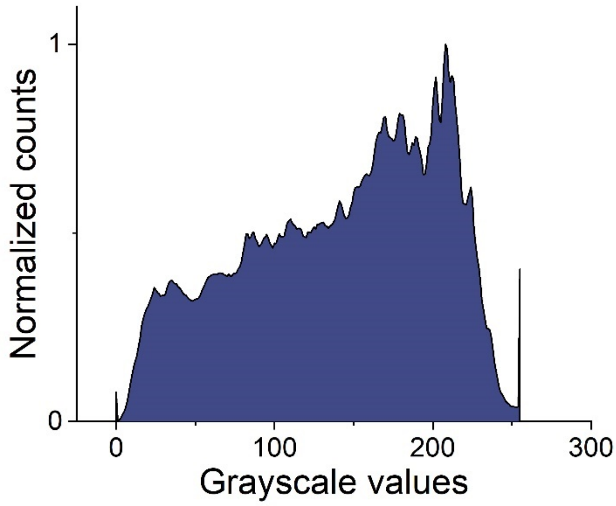


Fig. S21. Normalized brightness distributions of the 8-bit image.

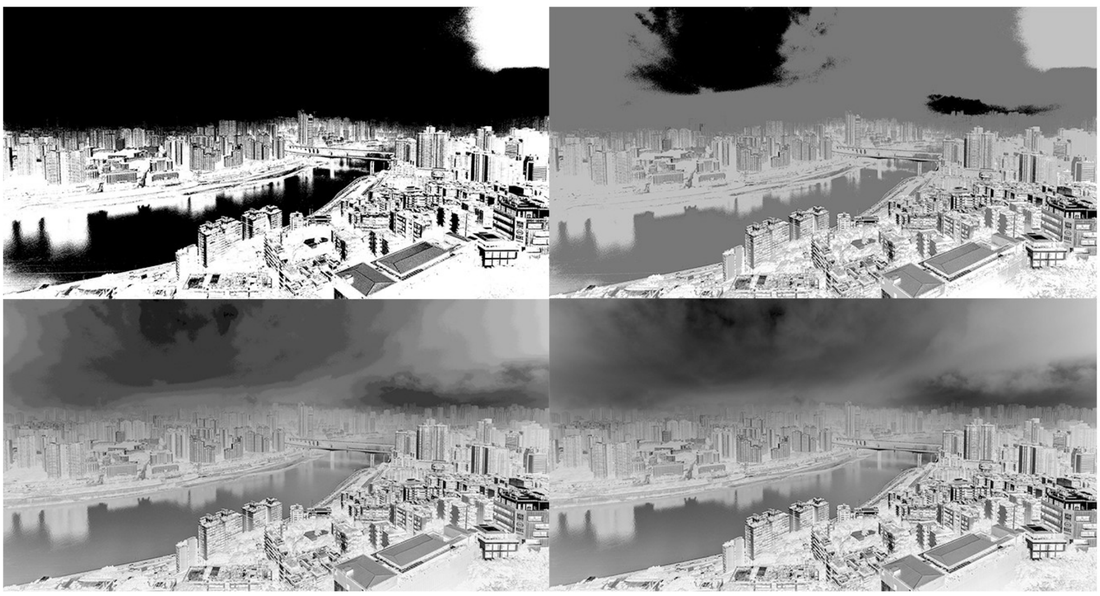


Fig. S22. Reversed 1-8 bit grayscale map.

9. Grayscale printing of GTA on PMMA pretreated DASA paper

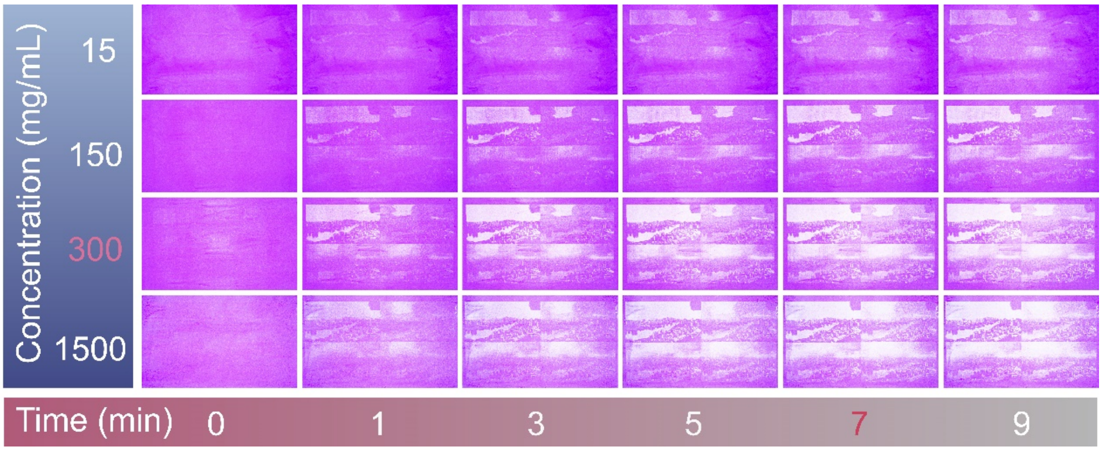


Fig. S23. Video screenshots of uniform exposure (10,000 lux) PMMA pretreated (0.02 g/mL) **DASA-MA** (1 mg/mL) paper printed with 15-1500 mg/mL **GTA**/EtOH ink at 0-9 min.

10. The relationships between grayscale bit depth and clarity

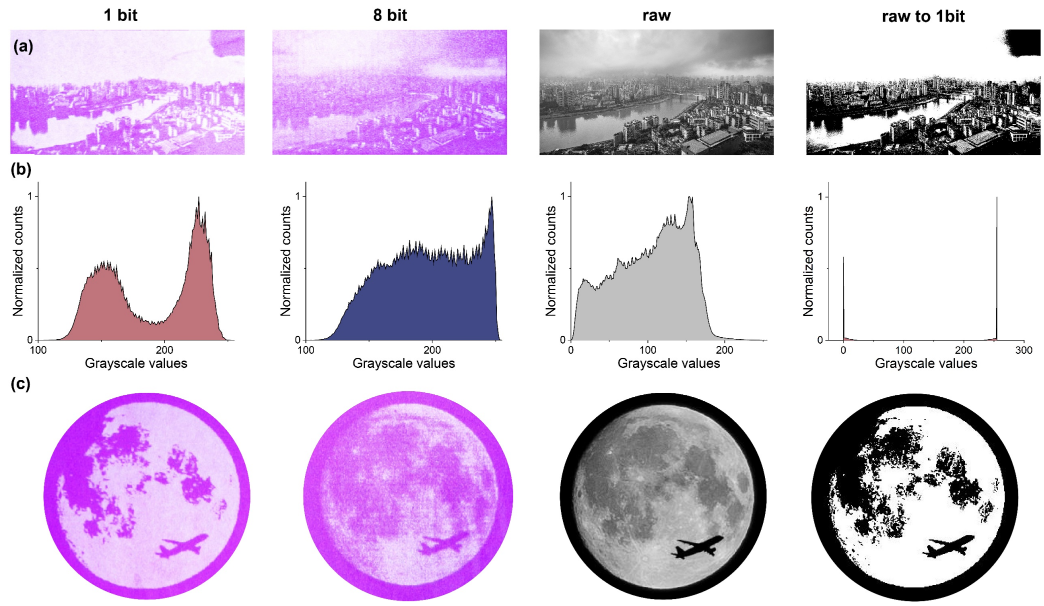


Fig. S24. (a) Video screenshots after white light exposure for 7 min and raw images for the 1-bit and 8-bit images, the photographic image of Chongqing was used; (b) Grayscale distribution plots of the video screenshots after white light exposure for 7 min and raw images for the 1-bit and 8-bit images. (c) Video screenshots after white light exposure for 7 min and raw images for the 1-bit and 8-bit images, the photographic image of lunar surface was used.

A trade-off exists between clarity and grayscale depth for the recording of grayscale images. The brightness of the images with low bit depth (1-bit) tends to locate in the lowest and highest regions, which results in a strong visual contrast to preserve the original images' outlines. However, these lead to a loss of grayscale details, such as the cloud formations in Fig. S24a and the brightness variations of lunar surface craters in Fig. S24c. This could be observed in the grayscale distribution, where both 1-bit images exhibit a significant gap between the bright and dark (Fig. S24b). Therefore, with the increase of grayscale depth, more detail could be recorded, while the clarity decreases.

11. The reversible isomerization of DASA-MA

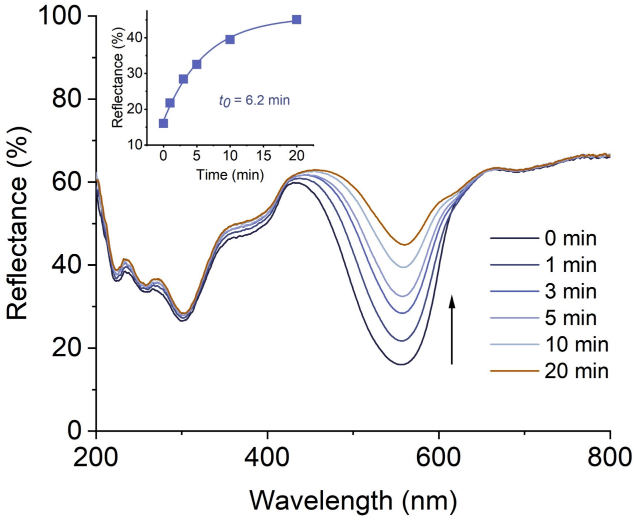


Fig. S25. Reflectance spectra of paper impregnated with **DASA-MA**/**GTA**/**PMMA**/DCM solution (1 mg/1 mg/20 mg/1 mL) over time upon green light irradiation (520 nm, 40 mW/cm^2), inner shows the time-dependent *linear*-to-*cyclic* isomerization of the above sample, the reflectance at 556 nm was monitored.

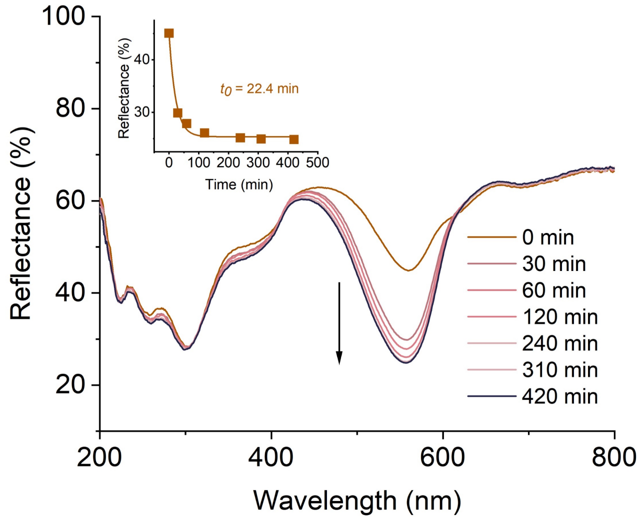


Fig. S26. Reflectance spectra of paper impregnated with **DASA-MA**/**GTA**/**PMMA**/DCM solution (1 mg/1 mg/20 mg/1 mL) over time under dark, the paper was pre-treated by 20 min green light irradiation (520 nm, 40 mW/cm^2), inner shows the time-dependent *cyclic*-to-*linear* isomerization of the above sample, the reflectance at 556 nm was monitored.

12. Crystal structure data for DASA-MA

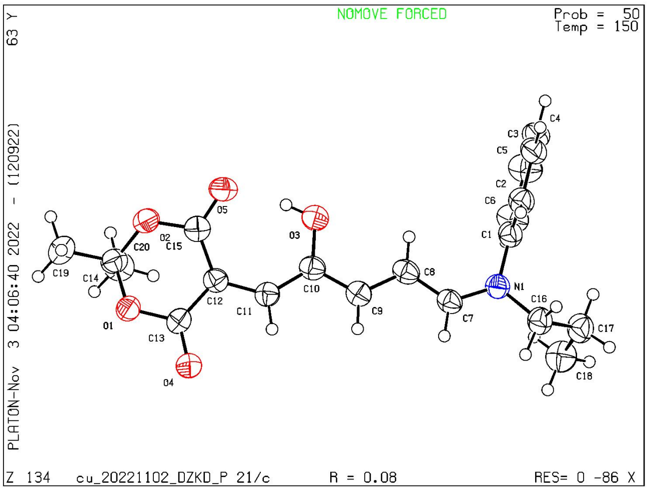


Fig. S27. Crystal structure data for **DASA-MA** could be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif CCDC# 2258697.

Table S1. Crystal data and structure refinement for **DASA-MA**.

CCDC number	2258697
Empirical formula	$C_{20}H_{23}NO_5$
Formula weight	357.39
Temperature [K]	150(2)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	9.87(3)
b [Å]	24.42(4)
c [Å]	7.70(2)
α [°]	90
β [°]	98.161(17)
γ [°]	90
Volume [Å^3]	1838(7)
Z	4
ρ_{calc} [gcm^{-3}]	1.292
μ [mm^{-1}]	0.763
F(000)	760
Crystal size [mm^3]	0.200×0.100×0.100
Crystal colour	red
Crystal shape	block
Radiation	CuK_α (λ=1.54184 Å)
2Θ range [°]	7.24 to 133.50 (0.84 Å)
Index ranges	-11 ≤ h ≤ 11
Reflections collected	10742
Independent reflections	3228
Completeness to	99.2 %
Data / Restraints /	3228/0/239
Goodness-of-fit on F^2	1.027
Final R indexes	R_1 = 0.0752
Final R indexes	R_1 = 0.1257
Largest peak/hole [eÅ^{-3}]	0.34/-0.27

Table S2. Atomic coordinates and Ueq [Å2] for **DASA-MA**.

Atom	***x***	***y***	***z***	***U*eq**
C12	0.9418(4)	0.40329(16)	0.8694(5)	0.0409(9)
C11	0.9046(4)	0.43328(16)	0.7143(5)	0.0413(9)
H11	0.941062	0.418721	0.616227	0.050
C13	1.0132(4)	0.35253(17)	0.8531(5)	0.0422(9)
N1	0.6427(3)	0.60183(13)	0.1970(4)	0.0432(8)
C7	0.7139(4)	0.56009(16)	0.2713(5)	0.0433(9)
H7	0.761826	0.538571	0.197223	0.052
C10	0.8260(4)	0.47962(16)	0.6751(5)	0.0442(9)
C9	0.8049(4)	0.49927(17)	0.5027(5)	0.0429(9)
H9	0.848057	0.480263	0.417817	0.052
C15	0.9278(4)	0.42212(17)	1.0428(5)	0.0449(9)
C1	0.5702(4)	0.63856(17)	0.2977(5)	0.0448(9)
O1	1.0526(3)	0.32243(11)	1.0022(4)	0.0457(7)
C8	0.7262(4)	0.54423(17)	0.4471(6)	0.0458(9)
H8	0.680700	0.564224	0.527589	0.055
C2	0.6325(4)	0.68667(17)	0.3600(6)	0.0494(10)
H2	0.721803	0.695463	0.336397	0.059
C14	0.9864(4)	0.33171(17)	1.1523(6)	0.0487(10)
O2	0.9707(3)	0.38921(12)	1.1816(4)	0.0504(7)
C16	0.6540(4)	0.61765(18)	0.0129(6)	0.0505(10)
H16A	0.710675	0.590106	-0.037756	0.061
H16B	0.701896	0.653275	0.013800	0.061
O5	0.8844(3)	0.46759(12)	1.0827(4)	0.0534(8)
C3	0.5631(5)	0.72202(18)	0.4575(6)	0.0551(11)
H3	0.606062	0.754689	0.504248	0.066
O4	1.0463(3)	0.33456(13)	0.7174(4)	0.0564(8)
O3	0.7615(3)	0.50708(13)	0.7937(4)	0.0572(8)
H3A	0.789446	0.495401	0.895140	0.086
C17	0.5177(5)	0.62234(19)	-0.1043(6)	0.0562(11)
H17A	0.458081	0.647766	-0.049498	0.067
H17B	0.532701	0.638207	-0.218314	0.067
C6	0.4389(4)	0.6263(2)	0.3274(7)	0.0577(12)
H6	0.396307	0.593372	0.282299	0.069
C4	0.4325(5)	0.7098(2)	0.4864(6)	0.0581(12)
H4	0.384865	0.734640	0.551096	0.070
C19	1.0817(6)	0.3102(2)	1.3048(6)	0.0618(12)
H19A	1.044181	0.317726	1.413554	0.093
H19B	1.170917	0.328047	1.309181	0.093
H19C	1.092453	0.270538	1.291778	0.093
C20	0.8479(5)	0.3042(2)	1.1251(7)	0.0617(12)
H20A	0.800071	0.312009	1.225483	0.093
H20B	0.859849	0.264602	1.114568	0.093
H20C	0.794098	0.318309	1.017640	0.093
C5	0.3695(5)	0.6621(2)	0.4231(7)	0.0648(13)
H5	0.279356	0.653854	0.444728	0.078
C18	0.4459(5)	0.5684(2)	-0.1362(7)	0.0647(13)
H18A	0.360925	0.573524	-0.217285	0.097
H18B	0.424516	0.553681	-0.024806	0.097
H18C	0.505289	0.542636	-0.187471	0.097

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S3. Bond lengths and angles for **DASA-MA**.

Atom–Atom	**Length [Å]**
C12–C11	1.405(6)
C12–C15	1.437(7)
C12–C13	1.440(6)
C11–C10	1.381(6)
C11–H11	0.9500
C13–O4	1.220(6)
C13–O1	1.372(5)
N1–C7	1.321(5)
N1–C1	1.441(6)
N1–C16	1.489(7)
C7–C8	1.397(7)
C7–H7	0.9500
C10–O3	1.361(5)
C10–C9	1.399(7)
C9–C8	1.378(6)
C9–H9	0.9500
C15–O5	1.244(5)
C15–O2	1.356(5)
C1–C2	1.380(6)
C1–C6	1.380(7)
O1–C14	1.425(6)
C8–H8	0.9500
C2–C3	1.387(7)
C2–H2	0.9500
C14–O2	1.434(6)
C14–C19	1.492(7)
C14–C20	1.510(7)
C16–C17	1.514(7)
C16–H16A	0.9900
C16–H16B	0.9900
C3–C4	1.373(8)
C3–H3	0.9500
O3–H3A	0.8400
C17–C18	1.500(7)
C17–H17A	0.9900
C17–H17B	0.9900
C6–C5	1.387(7)
C6–H6	0.9500
C4–C5	1.377(7)
C4–H4	0.9500
C19–H19A	0.9800
C19–H19B	0.9800
C19–H19C	0.9800
C20–H20A	0.9800
C20–H20B	0.9800
C20–H20C	0.9800
C5–H5	0.9500
C18–H18A	0.9800
C18–H18B	0.9800
C18–H18C	0.9800

Atom–Atom–Atom	**Angle [°]**
C11–C12–C15	125.1(4)
C11–C12–C13	116.5(4)
C15–C12–C13	118.0(3)
C10–C11–C12	133.1(4)
C10–C11–H11	113.4
C12–C11–H11	113.4
O4–C13–O1	116.4(4)
O4–C13–C12	125.3(4)
O1–C13–C12	118.2(4)
C7–N1–C1	121.4(4)
C7–N1–C16	120.4(4)
C1–N1–C16	117.4(3)
N1–C7–C8	127.0(4)
N1–C7–H7	116.5
C8–C7–H7	116.5
O3–C10–C11	124.0(4)
O3–C10–C9	116.6(4)
C11–C10–C9	119.4(4)
C8–C9–C10	124.7(4)
C8–C9–H9	117.7
C10–C9–H9	117.7
O5–C15–O2	114.5(4)
O5–C15–C12	126.6(4)
O2–C15–C12	118.8(4)
C2–C1–C6	120.7(4)
C2–C1–N1	119.1(4)
C6–C1–N1	120.3(4)
C13–O1–C14	119.0(3)
C9–C8–C7	119.3(4)
C9–C8–H8	120.4
C7–C8–H8	120.4
C1–C2–C3	119.2(4)
C1–C2–H2	120.4
C3–C2–H2	120.4
O1–C14–O2	110.9(3)
O1–C14–C19	105.8(4)
O2–C14–C19	107.0(4)
O1–C14–C20	109.1(4)
O2–C14–C20	109.9(4)

C19–C14–C20	114.2(4)
C15–O2–C14	119.0(3)
N1–C16–C17	114.0(4)
N1–C16–H16A	108.8
C17–C16–H16A	108.8
N1–C16–H16B	108.8
C17–C16–H16B	108.8
H16A–C16–H16B	107.6
C4–C3–C2	120.0(4)
C4–C3–H3	120.0
C2–C3–H3	120.0
C10–O3–H3A	109.5
C18–C17–C16	113.0(4)
C18–C17–H17A	109.0
C16–C17–H17A	109.0
C18–C17–H17B	109.0
C16–C17–H17B	109.0
H17A–C17–H17B	107.8
C1–C6–C5	119.9(4)
C1–C6–H6	120.1
C5–C6–H6	120.1
C3–C4–C5	120.9(4)
C3–C4–H4	119.5
C5–C4–H4	119.5
C14–C19–H19A	109.5
C14–C19–H19B	109.5
H19A–C19–H19B	109.5
C14–C19–H19C	109.5
H19A–C19–H19C	109.5
H19B–C19–H19C	109.5
C14–C20–H20A	109.5
C14–C20–H20B	109.5
H20A–C20–H20B	109.5
C14–C20–H20C	109.5
H20A–C20–H20C	109.5
H20B–C20–H20C	109.5
C4–C5–C6	119.3(5)
C4–C5–H5	120.4
C6–C5–H5	120.4
C17–C18–H18A	109.5
C17–C18–H18B	109.5
H18A–C18–H18B	109.5
C17–C18–H18C	109.5
H18A–C18–H18C	109.5
H18B–C18–H18C	109.5

Table S4. Torsion angles for **DASA-MA**.

Atom–Atom–Atom–Atom	**Torsion Angle [°]**
C15–C12–C11–C10	−14.6(7)
C13–C12–C11–C10	172.7(4)
C11–C12–C13–O4	1.9(6)
C15–C12–C13–O4	−171.3(4)
C11–C12–C13–O1	179.2(3)
C15–C12–C13–O1	6.0(5)
C1–N1–C7–C8	2.4(6)
C16–N1–C7–C8	172.2(4)
C12–C11–C10–O3	−1.1(7)
C12–C11–C10–C9	−178.4(4)
O3–C10–C9–C8	0.9(6)
C11–C10–C9–C8	178.5(4)
C11–C12–C15–O5	−1.8(7)
C13–C12–C15–O5	170.7(4)
C11–C12–C15–O2	−178.6(4)
C13–C12–C15–O2	−6.0(5)
C7–N1–C1–C2	95.3(5)
C16–N1–C1–C2	−74.8(5)
C7–N1–C1–C6	−86.3(5)
C16–N1–C1–C6	103.6(5)
O4–C13–O1–C14	−162.3(4)
C12–C13–O1–C14	20.1(5)
C10–C9–C8–C7	179.5(4)
N1–C7–C8–C9	179.9(4)
C6–C1–C2–C3	1.8(7)
N1–C1–C2–C3	−179.8(4)
C13–O1–C14–O2	−43.8(5)
C13–O1–C14–C19	−159.4(3)
C13–O1–C14–C20	77.4(5)
O5–C15–O2–C14	162.9(4)
C12–C15–O2–C14	−20.0(5)
O1–C14–O2–C15	43.8(5)
C19–C14–O2–C15	158.6(4)
C20–C14–O2–C15	−76.9(5)
C7–N1–C16–C17	127.8(4)
C1–N1–C16–C17	−61.9(5)
C1–C2–C3–C4	−2.0(7)
N1–C16–C17–C18	−67.0(5)
C2–C1–C6–C5	−1.1(7)
N1–C1–C6–C5	−179.4(4)
C2–C3–C4–C5	1.4(7)
C3–C4–C5–C6	−0.6(8)
C1–C6–C5–C4	0.4(8)

Table S5. Hydrogen bonds for **DASA-MA**.

D–H···A [Å]	**d(D–H) [Å]**	**d(H···A) [Å]**	**d(D···A) [Å]**	**<(DHA) [°]**
C7–H7···O5[#1]	0.95	2.36	3.278(7)	163.4
C2–H2···O4[#2]	0.95	2.49	3.349(10)	149.8
C16–H16A···O3[#1]	0.99	2.50	3.431(7)	157.4
C16–H16B···O1[#2]	0.99	2.52	3.263(9)	132.1
O3–H3A···O5	0.84	1.74	2.566(6)	165.6
C19–H19A···O4[#3]	0.98	2.37	3.299(10)	157.5
C19–H19C···O4[#4]	0.98	2.66	3.605(8)	163.5

Symmetry transformations used to generate equivalent atoms:

#1: +X, +Y, -1+Z; #2: 2-X, 1-Y, 1-Z; #3: +X, +Y, 1+Z; #4: +X, 0.5-Y, 0.5+Z;

13. NMR data and mass spectrum of DASA-MA

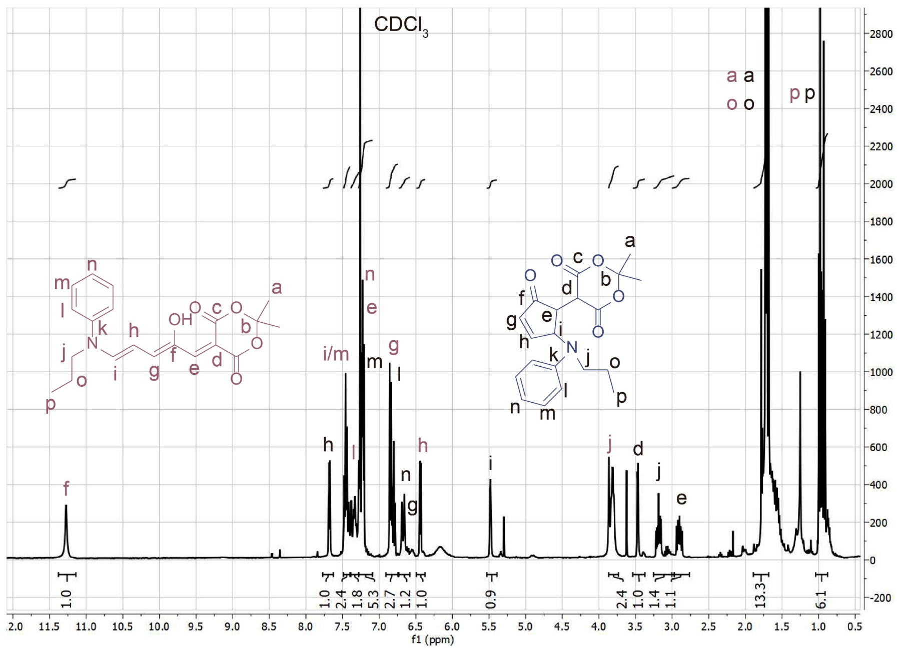


Fig. S28. ^{1}H NMR spectrum (400 MHz at 298 K) of **DASA-MA** ([**DASA-MA**]=10 mM in $CDCl_3$).

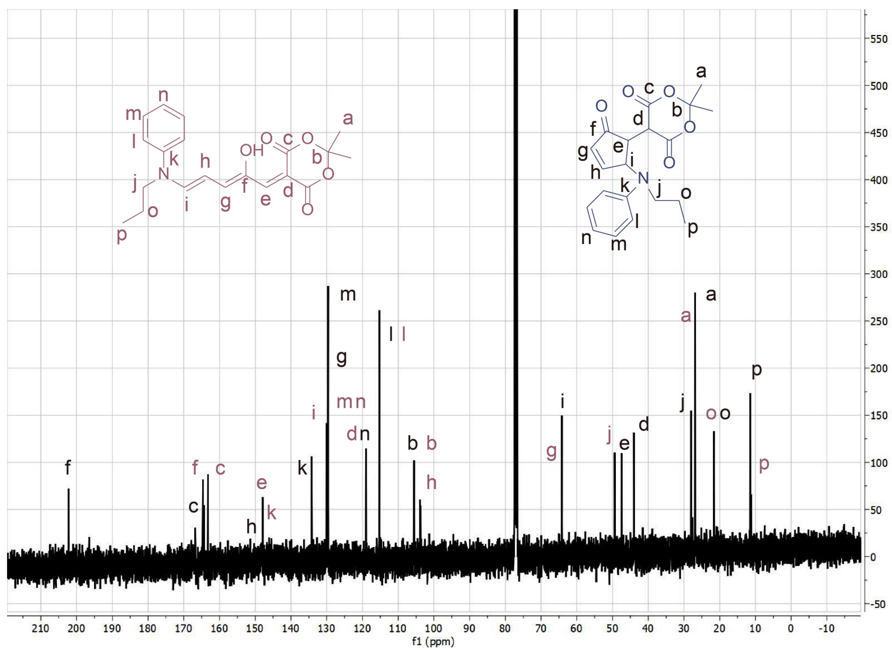


Fig. S29. ^{13}C NMR spectrum (100 MHz at 298 K) of **DASA-MA** ([**DASA-MA**]=10 mM in $CDCl_3$).

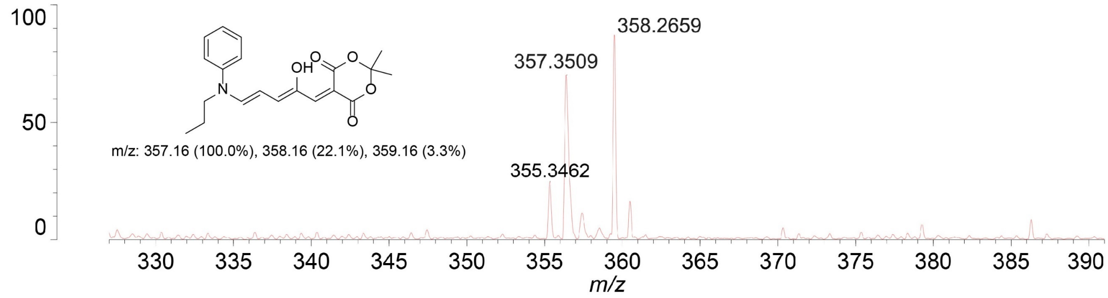


Fig. S30. Matrix-assisted laser ionization-time of flight (MALDI-TOF) mass spectrum of **DASA-MA**. m/z: M+ calcd. for 357.16, found 357.35.

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15. Calculated geometries:

In air

C	-2.04304	0.51654	1.09125
C	-2.26302	-0.65973	0.23275
C	-3.61306	-0.96467	-0.2208
O	-4.57232	-0.03377	0.02901
C	-4.18804	1.31812	0.32571
O	-3.1134	1.35232	1.26857
O	-1.0085	0.78557	1.65974
O	-3.97969	-2.00211	-0.7486
C	-5.38096	1.94929	1.01635
C	-3.78412	2.0351	-0.96017
C	-1.12908	-1.43118	-0.0081
C	-0.86687	-2.61797	-0.73066
C	0.44113	-3.09386	-0.83112
O	-1.81211	-3.40695	-1.29003
C	1.6701	-2.42835	-0.60101
C	1.86919	-1.07098	-0.71445
N	3.00523	-0.37808	-0.44767
C	2.99961	1.05167	-0.55168
C	4.18205	-1.03651	0.13869
C	4.06606	-1.24602	1.65423
C	5.30348	-1.93544	2.23202
C	1.97829	1.79766	0.04548
C	1.97715	3.18598	-0.07142
C	2.993	3.8388	-0.76515
C	4.0143	3.09346	-1.35296
C	4.018	1.7059	-1.25313
H	-5.6147	1.38879	1.92178
H	-5.15335	2.98107	1.28754
H	-6.24887	1.93349	0.35578
H	-3.51741	3.07001	-0.73944
H	-2.92521	1.55054	-1.42872
H	-4.61353	2.02482	-1.66919
H	-0.26353	-1.05263	0.51848
H	0.50543	-4.13486	-1.14193
H	4.3427	-1.98837	-0.37487
H	5.05129	-0.41597	-0.08125
H	3.9198	-0.27249	2.13294
H	3.17081	-1.83542	1.87251
H	5.20778	-2.07043	3.31179
H	5.45704	-2.92535	1.79099

H	6.21112	-1.35026	2.05409
H	1.19677	1.3073	0.61652
H	1.18207	3.75326	0.40079
H	2.99136	4.92054	-0.84726
H	4.80499	3.5918	-1.90425
H	4.796	1.12884	-1.74147
H	-2.70621	-3.04045	-1.10811
H	2.5194	-3.06818	-0.38241
H	1.07282	-0.45673	-1.11531

GTA

C	-1.11423	3.66001	-1.95161
O	-0.80048	3.54255	-3.35172
C	-0.85354	5.0836	-1.48518
C	-2.56307	3.23547	-1.80878
C	0.48018	3.30415	-3.69897
C	0.63236	3.26998	-5.18658
O	-1.60411	6.02142	-2.27589
C	-0.96697	6.585	-3.33343
C	-1.92097	7.40845	-4.1482
O	0.20368	6.42274	-3.57401
O	1.36088	3.12719	-2.88617
O	-2.68502	1.85792	-2.18325
C	-3.27913	1.58218	-3.38653
C	-3.1598	0.12567	-3.71345
O	-3.8039	2.4221	-4.06889
H	-0.46689	2.99269	-1.38415
H	-1.19325	5.21129	-0.4578
H	0.20689	5.31077	-1.55408
H	-2.86622	3.31027	-0.76409
H	-3.21313	3.84943	-2.42837
H	0.07756	4.09142	-5.63628
H	1.68247	3.32619	-5.45542
H	0.22336	2.33164	-5.56482
H	-2.5695	6.73313	-4.71097
H	-2.55641	8.01595	-3.50476
H	-1.36418	8.03416	-4.84047
H	-3.25414	-0.48711	-2.8184
H	-3.91699	-0.14173	-4.44638
H	-2.1692	-0.06326	-4.13615
C	-1.26296	-2.91887	-0.61637
C	0.1208	-2.90667	-0.21439
C	0.50604	-3.50087	1.06963

O	-0.52083	-3.97484	1.85097
C	-1.81207	-3.40408	1.67455
O	-2.16996	-3.38108	0.27834
O	-1.69511	-2.56068	-1.71614
O	1.63902	-3.63908	1.46494
C	-1.84825	-1.98543	2.22462
C	-2.79863	-4.33223	2.34426
C	1.16388	-2.34752	-0.94999
C	1.2753	-1.89511	-2.27613
C	2.43674	-1.23706	-2.68572
O	0.34798	-2.14827	-3.23558
C	3.33683	-0.56483	-1.8514
C	2.96454	-0.06709	-0.61796
N	3.76637	0.48102	0.31196
C	5.18203	0.34121	0.29143
C	3.12935	1.26307	1.38783
C	2.60262	2.62224	0.93265
C	1.92437	3.36489	2.07972
C	6.00281	1.45553	0.46086
C	7.38451	1.30338	0.47491
C	7.95472	0.04622	0.31294
C	7.13275	-1.06544	0.14762
C	5.7527	-0.92394	0.14252
H	-1.10471	-1.36066	1.72931
H	-2.83519	-1.55706	2.05552
H	-1.63155	-2.00556	3.29243
H	-3.80974	-3.94561	2.22217
H	-2.73419	-5.321	1.89303
H	-2.56691	-4.40778	3.40576
H	2.09879	-2.33658	-0.40652
H	2.61981	-1.22325	-3.75547
H	-0.50099	-2.41674	-2.80552
H	4.33733	-0.366	-2.21668
H	1.91166	-0.02407	-0.36411
H	2.30096	0.66811	1.77878
H	3.86234	1.37366	2.1859
H	3.42172	3.22157	0.52667
H	1.88688	2.473	0.12317
H	1.4842	4.2983	1.72896
H	1.12357	2.75761	2.50827
H	2.63058	3.59696	2.88106
H	5.56388	2.43766	0.57038
H	8.01508	2.17389	0.60374
H	9.0308	-0.06882	0.32069

H	7.56677	-2.05108	0.03813
H	5.11182	-1.78884	0.03882

HH

C	1.92061	-0.89249	-1.21187
C	0.56426	-1.34644	-0.97192
C	0.34871	-2.60814	-0.24923
O	1.45393	-3.16892	0.33215
C	2.57004	-2.32083	0.60654
O	2.90901	-1.55702	-0.56488
O	2.26209	-0.01728	-1.99434
O	-0.71332	-3.17757	-0.14196
C	3.75103	-3.22548	0.87127
C	2.25541	-1.38586	1.76642
C	-0.59281	-0.71704	-1.41051
C	-0.85873	0.50456	-2.05477
C	-2.16935	0.95982	-2.18107
O	0.09094	1.29632	-2.60914
C	-3.32113	0.54438	-1.4885
C	-3.31362	-0.09836	-0.27458
N	-4.36963	-0.61851	0.38111
C	-5.64579	-0.77603	-0.23396
C	-4.17794	-1.07737	1.76663
C	-4.03426	0.05239	2.78445
C	-3.7957	-0.48902	4.19166
C	-6.77887	-0.22002	0.35567
C	-8.02578	-0.40526	-0.23114
C	-8.14455	-1.13369	-1.40901
C	-7.00954	-1.6858	-1.99691
C	-5.76304	-1.51382	-1.41145
H	3.92763	-3.85852	0.00328
H	4.63932	-2.62538	1.06513
H	3.54452	-3.85335	1.73679
H	3.1077	-0.73904	1.96245
H	1.4003	-0.75155	1.53751
H	2.03092	-1.9767	2.65376
H	-1.47482	-1.30884	-1.21671
H	-2.29583	1.76964	-2.89285
H	0.97419	0.85562	-2.5321
H	-4.27948	0.8062	-1.92025
H	-2.38434	-0.17677	0.27394
H	-5.02843	-1.71041	2.01552
H	-3.28738	-1.71346	1.78481

H	-3.20585	0.69941	2.48741
H	-4.93097	0.67655	2.76719
H	-3.68748	0.32451	4.91011
H	-4.62699	-1.11659	4.52204
H	-2.88664	-1.09362	4.23315
H	-6.68261	0.36331	1.26141
H	-8.90308	0.03041	0.2297
H	-9.11554	-1.27308	-1.86623
H	-7.0961	-2.26391	-2.90799
H	-4.87905	-1.95299	-1.85397
C	9.07818	2.74546	-1.90702
C	7.66455	2.18448	-2.0477
C	6.66317	3.21149	-2.57376
C	5.24631	2.65861	-2.71504
C	4.27371	3.70538	-3.24157
C	2.84956	3.21836	-3.33655
O	2.07096	4.12245	-3.97398
C	0.65678	3.82446	-4.00232
C	-0.05436	4.97671	-4.67799
C	-1.56848	4.77128	-4.69325
C	-2.31708	5.90978	-5.38156
C	-3.836	5.78754	-5.281
C	-4.57779	6.96277	-5.91451
O	2.43138	2.17471	-2.90167
H	9.77281	1.99219	-1.52959
H	9.45935	3.09704	-2.86952
H	9.09766	3.59191	-1.21549
H	7.31908	1.81181	-1.07802
H	7.67755	1.31941	-2.71889
H	7.00952	3.58575	-3.54498
H	6.64861	4.0774	-1.90124
H	4.89006	2.29499	-1.74861
H	5.25038	1.79122	-3.38117
H	4.57802	4.06709	-4.22834
H	4.25591	4.58052	-2.58692
H	0.5021	2.88586	-4.53809
H	0.30744	3.69017	-2.97869
H	0.18027	5.90109	-4.14364
H	0.32451	5.09185	-5.69831
H	-1.80812	3.82566	-5.19196
H	-1.92026	4.67747	-3.66214
H	-2.0106	6.85743	-4.93154
H	-2.02233	5.96135	-6.43624
H	-4.15501	4.85172	-5.7513

H	-4.11453	5.70961	-4.2256
H	-5.66012	6.82992	-5.85792
H	-4.33073	7.89698	-5.40632
H	-4.31052	7.07658	-6.96863

HB

C	-1.83318	0.83286	-1.44038
C	-0.50618	1.3667	-1.18591
C	-0.38162	2.68516	-0.54461
O	-1.53946	3.22638	-0.05519
C	-2.60652	2.33172	0.26716
O	-2.87188	1.45934	-0.84808
O	-2.1006	-0.10098	-2.18431
O	0.64493	3.31513	-0.44159
C	-3.85016	3.16884	0.44432
C	-2.25238	1.50991	1.49834
C	0.69198	0.75873	-1.52692
C	1.0305	-0.45617	-2.15924
C	2.35717	-0.87253	-2.20424
O	0.14391	-1.24918	-2.80543
C	3.43222	-0.4456	-1.40278
C	3.28887	0.11553	-0.15909
N	4.25691	0.63924	0.62385
C	5.55725	0.94785	0.13618
C	3.93602	0.89611	2.03606
C	3.8165	-0.36792	2.88569
C	3.45664	-0.04053	4.33243
C	6.68717	0.51875	0.83136
C	7.95505	0.85721	0.37241
C	8.10417	1.61302	-0.78426
C	6.97433	2.0396	-1.47746
C	5.70529	1.71568	-1.01994
H	-4.04981	3.722	-0.47195
H	-4.69757	2.52401	0.66786
H	-3.70417	3.87202	1.26316
H	-3.06077	0.81846	1.71861
H	-1.34231	0.93356	1.33579
H	-2.09873	2.17887	2.34443
H	1.5475	1.37155	-1.28067
H	2.56457	-1.65168	-2.93085
H	-0.76394	-0.85811	-2.731
H	4.43456	-0.63533	-1.76755
H	2.31283	0.1046	0.30909

H	4.70947	1.55361	2.43013
H	2.99527	1.45468	2.06642
H	3.05689	-1.02068	2.44978
H	4.75577	-0.925	2.84597
H	3.36242	-0.94962	4.92776
H	4.22005	0.58619	4.79995
H	2.50613	0.49542	4.3909
H	6.57605	-0.08575	1.72122
H	8.82712	0.5186	0.91719
H	9.09213	1.87178	-1.1422
H	7.08033	2.64126	-2.3711
H	4.82586	2.06354	-1.54444
C	-3.68064	-3.79546	-3.32239
C	-3.90413	-3.53979	-1.96996
C	-4.93178	-4.18903	-1.29993
C	-5.75411	-5.08283	-1.98111
C	-5.54324	-5.32809	-3.33458
C	-4.50443	-4.69196	-4.00348
C	-2.57271	-3.06704	-4.00269
O	-2.12582	-3.73092	-5.08891
C	-1.03146	-3.11712	-5.81055
C	-0.41756	-4.17133	-6.70661
C	0.75018	-3.61804	-7.52237
C	1.3973	-4.67405	-8.4159
C	2.63085	-4.16723	-9.1601
C	3.27757	-5.22819	-10.04828
O	-2.13117	-2.00809	-3.63001
H	-3.25967	-2.83624	-1.46083
H	-5.0938	-3.99797	-0.24675
H	-6.55922	-5.58463	-1.45899
H	-6.18754	-6.01552	-3.86816
H	-4.335	-4.87554	-5.05536
H	-1.42613	-2.27659	-6.38647
H	-0.31155	-2.73358	-5.09075
H	-0.06509	-4.998	-6.08395
H	-1.18527	-4.57846	-7.37204
H	0.40478	-2.78247	-8.14109
H	1.50208	-3.21465	-6.83898
H	1.6836	-5.53102	-7.79957
H	0.66133	-5.04623	-9.13862
H	2.35376	-3.29839	-9.76606
H	3.36165	-3.80907	-8.42861
H	4.14038	-4.82798	-10.5847
H	3.62049	-6.07723	-9.4539

H	2.5695	-5.60506	-10.79142

TGD

C	0.50572	-0.21423	-1.74565
C	-0.65217	-1.0167	-1.43454
C	-0.48012	-2.271	-0.69322
O	0.7797	-2.51688	-0.20865
C	1.63847	-1.40125	0.01273
O	1.67792	-0.56215	-1.16159
O	0.54139	0.74417	-2.51239
O	-1.34255	-3.09632	-0.50393
C	3.03581	-1.95434	0.17579
C	1.15737	-0.58502	1.20536
C	-1.96507	-0.69587	-1.75868
C	-2.56627	0.33359	-2.50736
C	-3.95472	0.4689	-2.48534
O	-1.89086	1.18747	-3.31474
C	-4.78307	0.03004	-1.44296
C	-4.29326	-0.12788	-0.16215
N	-4.92178	-0.67465	0.89414
C	-6.09921	-1.46454	0.76807
C	-4.32485	-0.46895	2.22444
C	-4.48295	0.95448	2.75453
C	-3.76642	1.13739	4.0896
C	-7.21606	-1.19112	1.55571
C	-8.34896	-1.99038	1.45315
C	-8.37698	-3.05609	0.5611
C	-7.25885	-3.32777	-0.22308
C	-6.12034	-2.54145	-0.11883
H	3.29039	-2.55499	-0.69597
H	3.75469	-1.14179	0.26529
H	3.07907	-2.58112	1.06563
H	1.82909	0.25397	1.3797
H	0.15668	-0.18834	1.03081
H	1.13419	-1.22161	2.08941
H	-2.66913	-1.42891	-1.39243
H	-4.40008	1.00741	-3.31594
H	-0.91667	1.05022	-3.18573
H	-5.83757	-0.13059	-1.63334
H	-3.32218	0.29411	0.07186
H	-4.78063	-1.18966	2.90182
H	-3.2623	-0.71637	2.15149
H	-4.07102	1.64736	2.01778

H	-5.54544	1.1913	2.85725
H	-3.88727	2.15529	4.46294
H	-4.15671	0.45564	4.84948
H	-2.69609	0.94611	3.98532
H	-7.20161	-0.35183	2.23801
H	-9.2138	-1.77176	2.06656
H	-9.26111	-3.67505	0.48044
H	-7.26587	-4.1662	-0.90776
H	-5.24031	-2.76451	-0.70684
C	2.22228	3.61443	-3.9345
C	0.92857	3.24155	-4.595
O	0.79483	3.85373	-5.78681
C	-0.45042	3.69341	-6.49808
C	-1.30293	4.93129	-6.28921
O	-2.54128	4.68533	-6.93372
C	-3.50056	5.70791	-6.70263
C	-4.80135	5.24304	-7.3262
O	-5.82491	6.11937	-6.89016
C	-7.09911	5.78169	-7.40114
C	-8.0849	6.77683	-6.82826
O	-9.37733	6.41038	-7.34876
C	-10.41831	7.18395	-6.96119
C	-11.7052	6.69627	-7.5691
O	0.09348	2.50038	-4.12202
O	-10.30021	8.13068	-6.22631
H	2.0524	4.52295	-3.3509
H	2.52766	2.8263	-3.25057
H	2.99665	3.81338	-4.67244
H	-0.18534	3.56895	-7.54618
H	-0.97108	2.8083	-6.14028
H	-1.44745	5.11472	-5.22081
H	-0.80898	5.81259	-6.717
H	-3.64144	5.86703	-5.62943
H	-3.17442	6.65442	-7.14987
H	-4.73021	5.2412	-8.42107
H	-5.01077	4.21485	-7.00298
H	-7.10621	5.82959	-8.49775
H	-7.379	4.76157	-7.10633
H	-8.09662	6.73514	-5.73891
H	-7.83639	7.79458	-7.1292
H	-11.63263	6.71236	-8.65758
H	-11.89167	5.66428	-7.26832
H	-12.52318	7.33203	-7.24191