

## Electronic Supplementary Information

### Room-Temperature Photosynthesis of Zn(I) Compounds with High Air Stability

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#### Index:

<b>Tables</b> .....	S1
<b>Table S1.</b> Crystal structure refinement data for <b>2</b> . .....	S1
<b>Table S2.</b> Selected bond lengths [Å] and angles [°] for <b>1</b> before coloration.....	S2
<b>Table S3.</b> Selected bond lengths [Å] and angles [°] for <b>2</b> before coloration.....	S2
<b>Table S4.</b> Selected hydrogen bond lengths [Å] for <b>1</b> and <b>2</b> . .....	S3
<b>Figures</b> .....	S4
<b>Figure S1.</b> TGA and DSC curves of <b>2</b> in nitrogen atmosphere. ....	S4
<b>Figure S2.</b> Experimental and simulated PXRD patterns for <b>1</b> . .....	S4
<b>Figure S3.</b> Experimental and simulated PXRD patterns for <b>2</b> . .....	S5
<b>Figure S4.</b> IR spectra of <b>1</b> before and after irradiation. ....	S5
<b>Figure S5.</b> IR spectra of <b>2</b> before and after irradiation. ....	S6
<b>Figure S6.</b> Optical density difference of <b>2</b> .....	S6
<b>Figure S7.</b> Optical density difference of <b>2</b> .....	S7
<b>Figure S8.</b> Time-dependent UV-vis data of <b>1</b> and <b>2</b> at 369 and 355 nm, respectively. ....	S7
<b>Figure S9.</b> UV-vis data of <b>1</b> using different light sources. ....	S8
<b>Figure S10.</b> UV-vis data of <b>2</b> using different light sources. ....	S8

## Tables

**Table S1.** Crystal structure refinement data for **2**.

Chemical formula	$[\text{Zn}_2(\text{PA})_4(\text{bipy})]_n$ ( <b>2</b> )
CCDC	2244456
Formula weight	579.20
Temperature (K)	293(2)
Space group	<i>Pnma</i>
<i>a</i> /Å	16.7620(5)
<i>b</i> /Å	10.6688(5)
<i>c</i> /Å	14.1832(4)
$\alpha$ /°	90
$\beta$ /°	90
$\gamma$ /°	90
Volume/Å <sup>3</sup>	2536.39(16)
<i>Z</i>	4
<i>D<sub>c</sub></i> /g cm <sup>-3</sup>	1.517
$\mu$ /mm <sup>-1</sup>	2.737
<i>F</i> (000)	1192.0
GOF on <i>F</i> <sup>2</sup>	1.086
<i>R</i> <sub>1</sub> <sup>a</sup> ( <i>I</i> >2σ( <i>I</i> ))	0.0472
<i>wR</i> <sub>2</sub> <sup>b</sup> ( <i>I</i> >2σ( <i>I</i> ))	0.1531
<i>R</i> <sub>1</sub> <sup>a</sup> (all data)	0.0514
<i>wR</i> <sub>2</sub> <sup>b</sup> (all data)	0.1580

$$^a R_1 = \sum(F_o - F_c)/\sum F_o; \quad ^b wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$$

**Table S2.** Selected bond lengths [Å] and angles [°] for **1** before coloration.

Bond	Length/Å	Angle	Angle/°
Zn2-O12	2.3459(15)	O22-Zn2-N1 <sup>1</sup>	94.18(6)
Zn2-O32	1.9972(13)	O42-Zn2-N1 <sup>1</sup>	91.79(6)
Zn2-O42	2.2396(15)	O12-Zn1-N2	123.96(6)
Zn2-O22	2.0207(15)	N2-Zn1-O31	100.75(6)
Zn2-O41	2.0843(14)	N2-Zn1-O21	104.97(6)
Zn2-N1 <sup>1</sup>	2.1682(16)	O32-Zn2-N1 <sup>1</sup>	90.60(6)
Zn1-O12	2.0082(14)	O41-Zn2-N1 <sup>1</sup>	91.65(6)
Zn1-O21	1.9488(15)	O22-Zn2-N1 <sup>1</sup>	94.18(6)
Zn1-O31	1.9815(14)	N11-Zn2-O12	170.46(6)
Zn1-O11	2.4750(15)		
N2-Zn1	2.0268(15)		

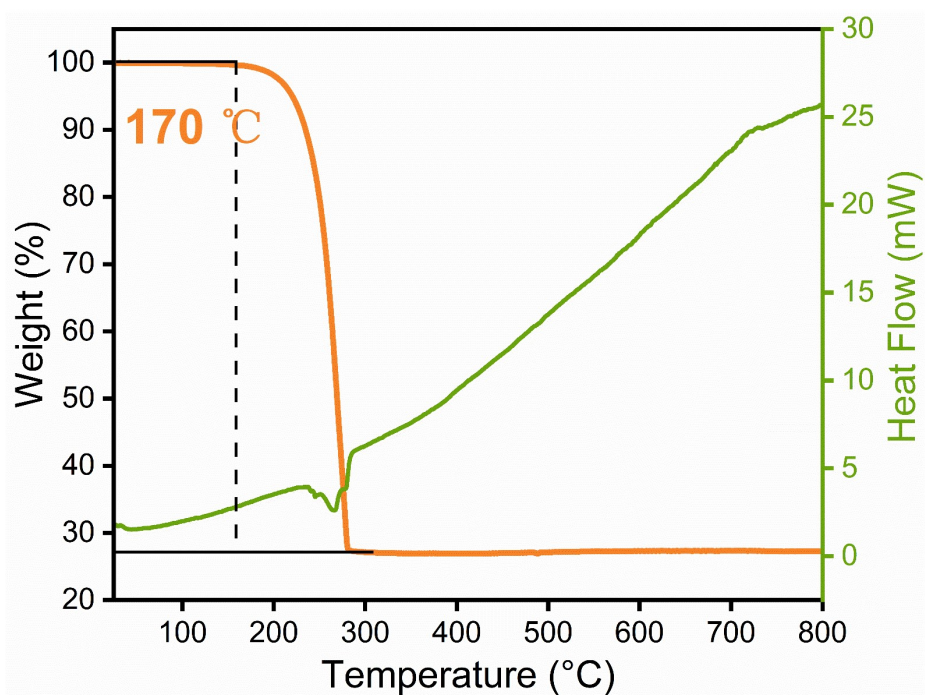
**Table S3.** Selected bond lengths [Å] and angles [°] for **2** before coloration.

Bond	Length/Å	Angle	Angle/°
Zn1-N11 <sup>1</sup>	2.030(3)	N11 <sup>1</sup> -Zn1-O41	85.90(19)
Zn1-O31	1.940(3)	N11 <sup>1</sup> -Zn1-O41 <sup>2</sup>	85.90(19)
Zn1-O31 <sup>2</sup>	1.940(3)	O31 <sup>2</sup> -Zn1-N11 <sup>1</sup>	101.90(10)
Zn1-O41	2.417(7)	O31-Zn1-N11 <sup>1</sup>	101.90(10)
Zn1-O41 <sup>2</sup>	2.417(7)	O42-Zn1-N11 <sup>1</sup>	132.72(17)
Zn1-O42	1.989(4)	N12-Zn2-O21	86.53(11)
Zn2-N12	2.174(3)	N12-Zn2-O21 <sup>2</sup>	86.53(11)
Zn2-O21 <sup>2</sup>	2.181(2)	N12-Zn2-O42	179.88(14)
Zn2-O21	2.181(2)	O32-Zn2-N12	90.08(9)
Zn2-O32	2.011(2)	O32 <sup>2</sup> -Zn2-N12	90.08(9)
Zn2-O32 <sup>2</sup>	2.011(2)		
Zn2-O42	2.202(4)		

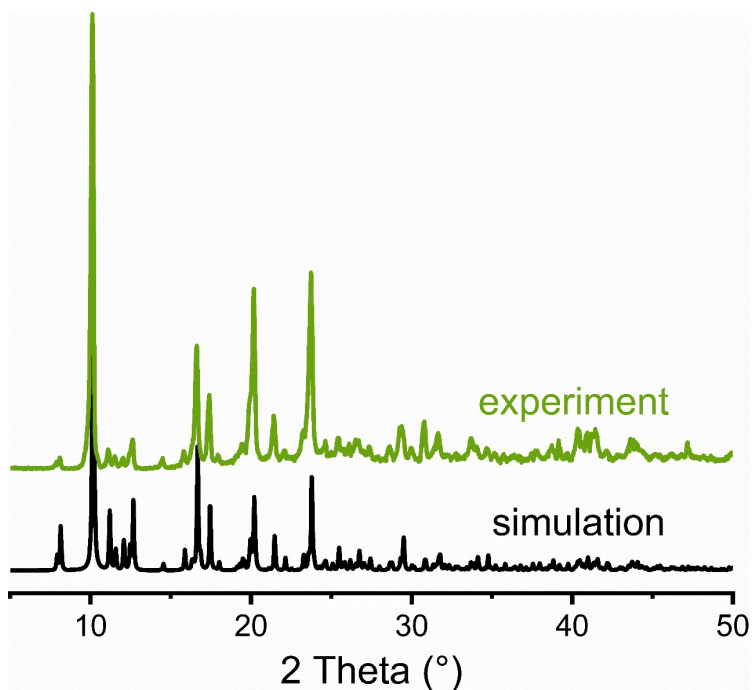
Symmetry codes: <sup>1</sup>+X, +Y, 1+Z; <sup>2</sup>+X, 3/2-Y, +Z; <sup>1</sup>+X, +Y, 1+Z; <sup>2</sup>+X, 3/2-Y, +Z; <sup>3</sup>+X, +Y, -1+Z.

**Table S4.** Selected hydrogen bond lengths [ $\text{\AA}$ ] for **1** and **2**.

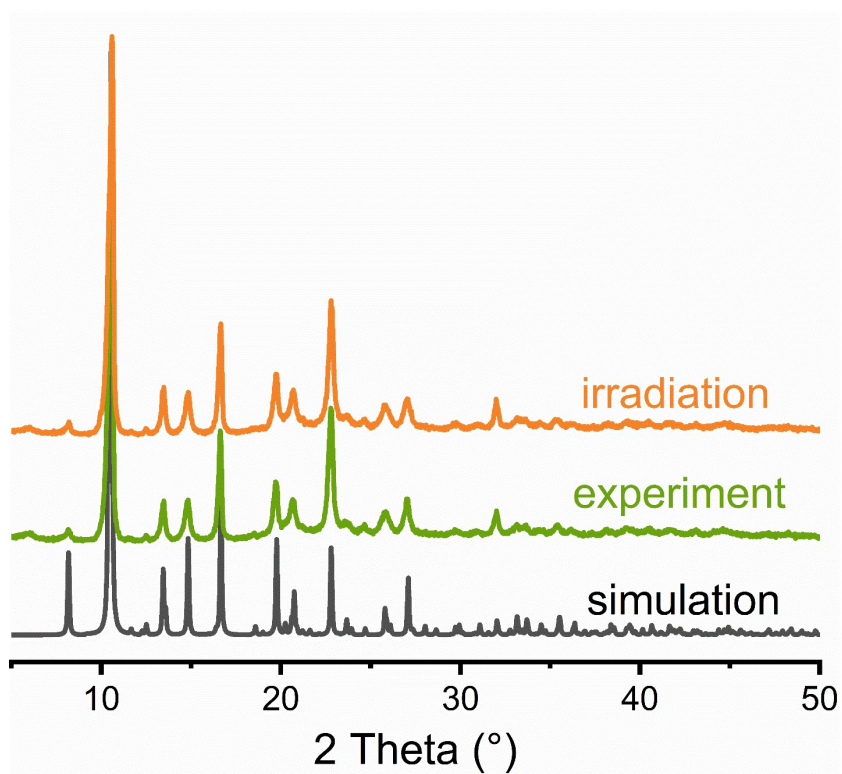
<b><math>[\text{Zn}_2(\text{MAA})_4(\text{bipy})]_n</math> (1)</b>		<b><math>[\text{Zn}_2(\text{PA})_4(\text{bipy})]_n</math> (2)</b>	
<b>Bond</b>	<b>Length/<math>\text{\AA}</math></b>	<b>Bond</b>	<b>Length/<math>\text{\AA}</math></b>
$d_{1(\text{H}\cdots\text{O})}: \text{C2-H}_{\text{bipy}}\cdots\text{O41}_{\text{MAA}}$	2.486	$d_{6(\text{H}\cdots\text{O})}: \text{C15-H}_{\text{bipy}}\cdots\text{O21}_{\text{PA}}$	2.379
$d_{2(\text{H}\cdots\text{O})}: \text{C2-H}_{\text{bipy}}\cdots\text{O22}_{\text{MAA}}$	3.429	$d_{7(\text{H}\cdots\text{O})}: \text{C12-H}_{\text{bipy}}\cdots\text{O21}_{\text{PA}}$	2.629
$d_{3(\text{H}\cdots\text{O})}: \text{C5-H}_{\text{bipy}}\cdots\text{O22}_{\text{MAA}}$	3.070	$d_{8(\text{H}\cdots\text{O})}: \text{C12-H}_{\text{bipy}}\cdots\text{O32}_{\text{PA}}$	3.033
$d_{4(\text{H}\cdots\text{O})}: \text{C6-H}_{\text{bipy}}\cdots\text{O11}_{\text{MAA}}$	3.884	$d_{9(\text{H}\cdots\text{O})}: \text{C11-H}_{\text{bipy}}\cdots\text{O31}_{\text{PA}}$	3.536
$d_{5(\text{H}\cdots\text{O})}: \text{C6-H}_{\text{bipy}}\cdots\text{O21}_{\text{MAA}}$	2.420	$d_{10(\text{H}\cdots\text{O})}: \text{C11-H}_{\text{bipy}}\cdots\text{O41}_{\text{PA}}$	2.598



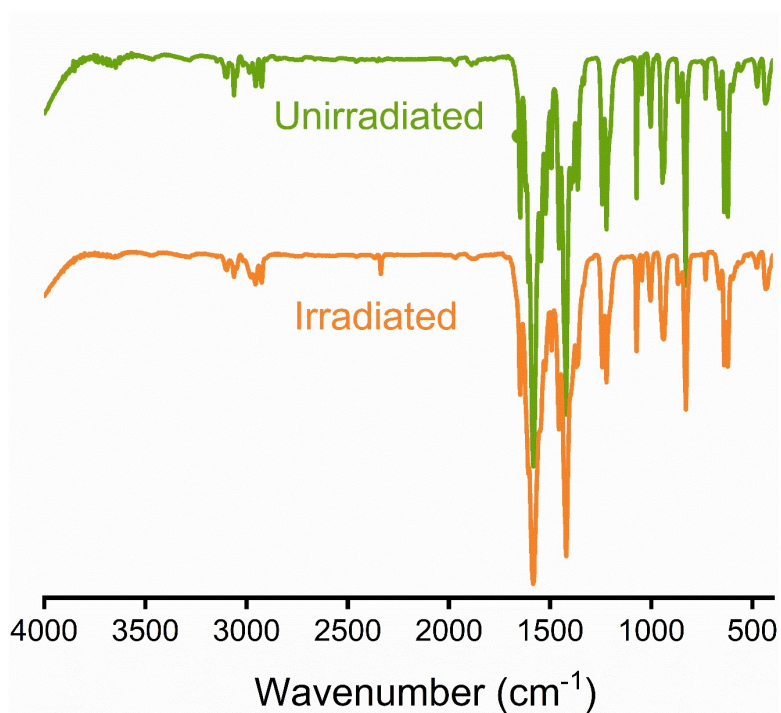
**Figure S1.** TGA and DSC curves of **2** in nitrogen atmosphere with the ramp rate of 10 °C/min.



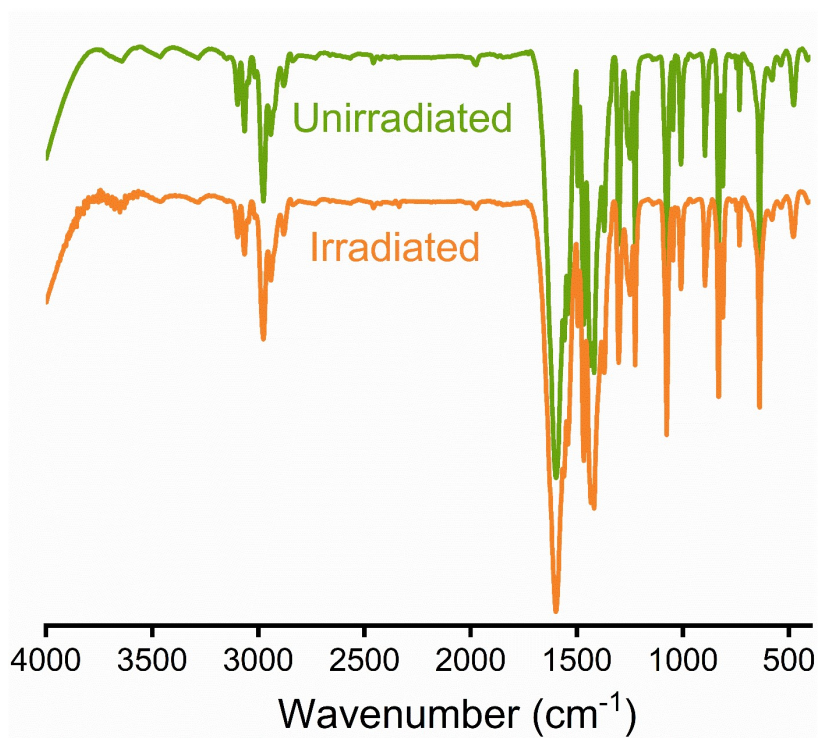
**Figure S2.** Experimental and simulated PXRD patterns for **1**. The time for irradiation-treatment was 30 min.



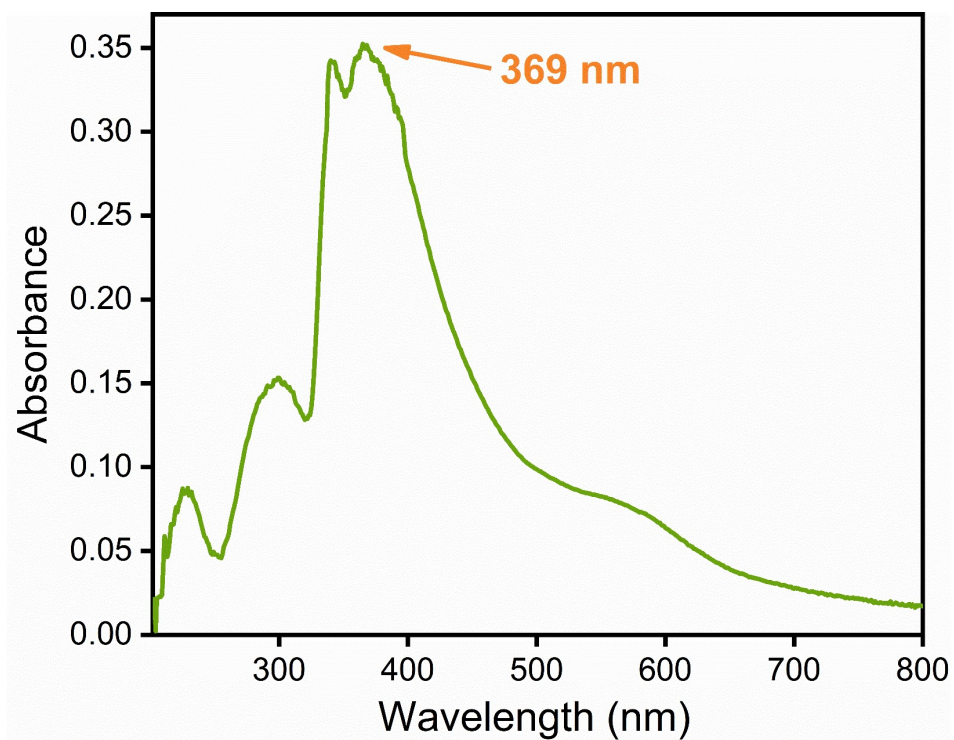
**Figure S3.** Experimental and simulated PXRD patterns for **2**. The time for irradiation-treatment was 30 min.



**Figure S4.** IR spectra of **1** before and after irradiation. The time for irradiation-treatment was 30 min.



**Figure S5.** IR spectra of **2** before and after irradiation. The time for irradiation-treatment was 30 min.



**Figure S6.** Optical density difference of **2**. The time for irradiation-treatment was 30 min.

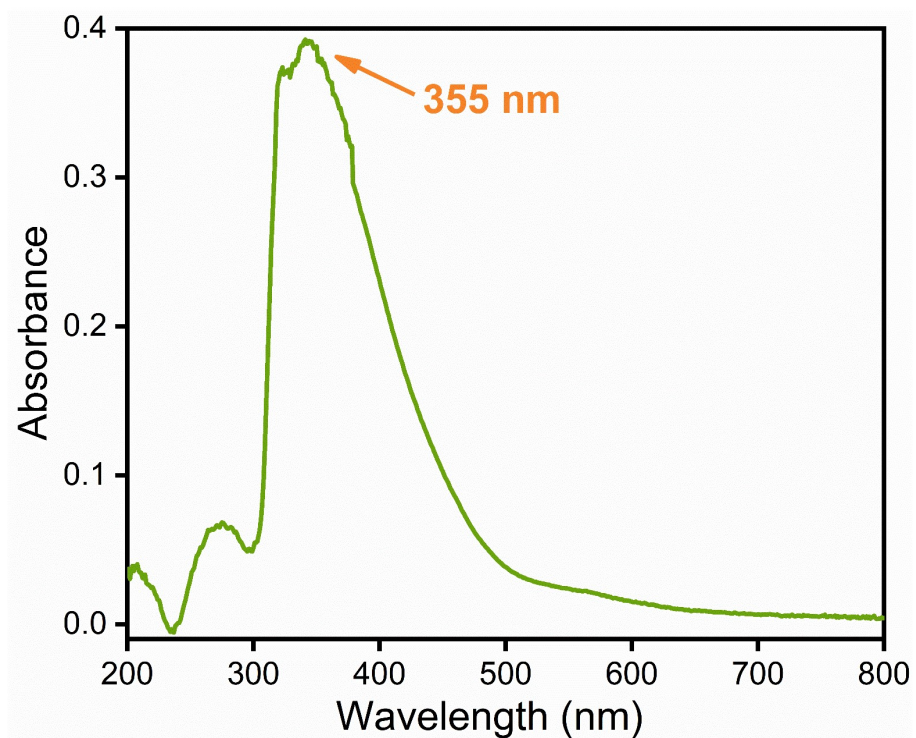


Figure S7. Optical density difference of **2**. The time for irradiation-treatment was 30 min.

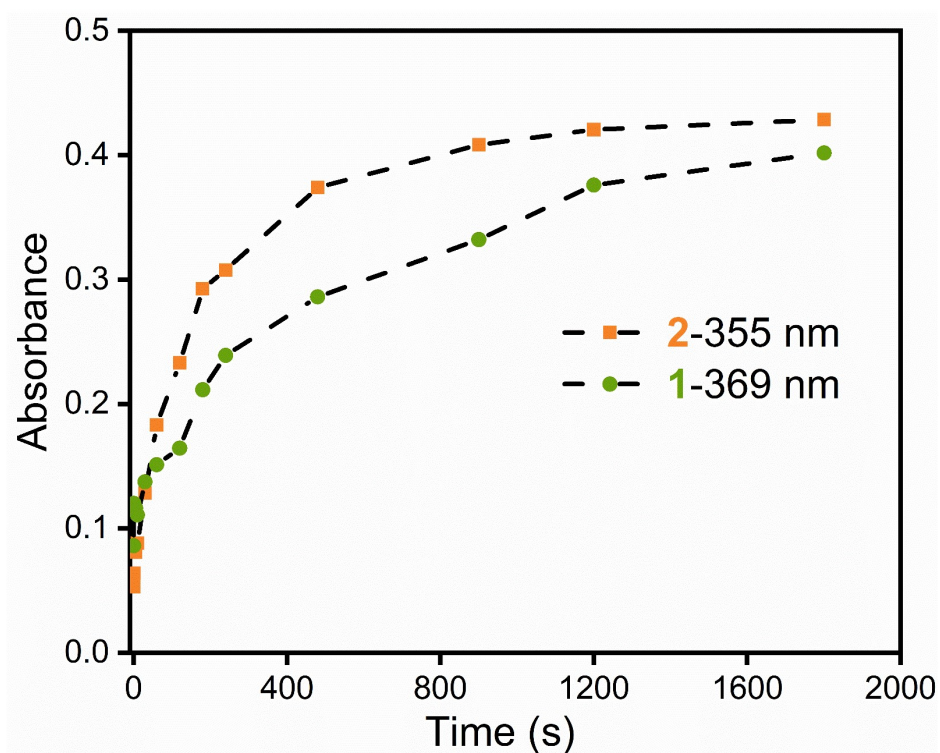


Figure S8. Time-dependent UV-vis data of **1** and **2** monitored at 369 and 355 nm, respectively.



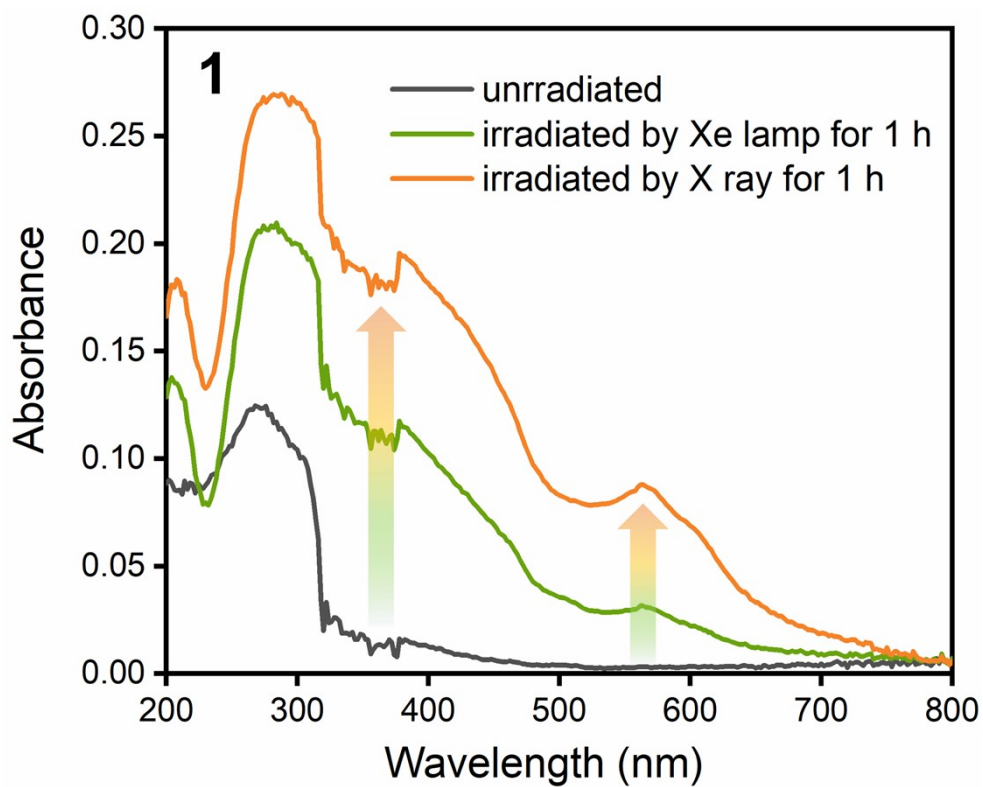


Figure S9. UV-vis data of **1** using different light sources.

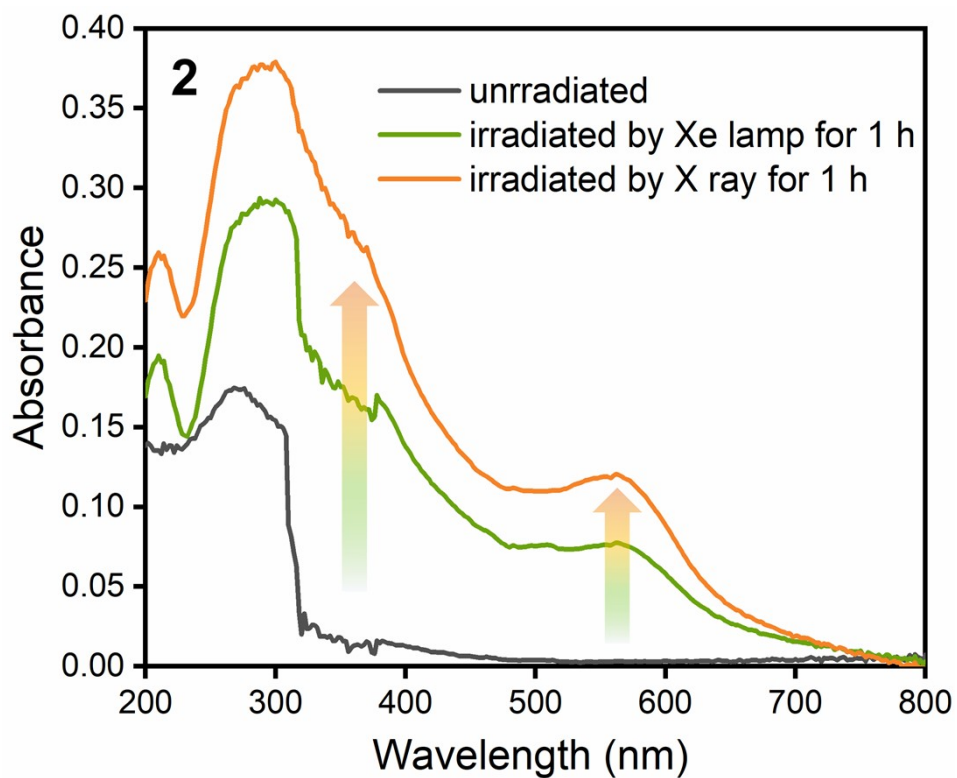


Figure S10. UV-vis data of **2** using different light sources.