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Reporting Summary

Nature Portfolio wishes to improve the reproducibility of the work that we publish. This form provides structure for consistency and transparency in reporting. For further information on Nature Portfolio policies, see our Editorial Policies and the Editorial Policy Checklist.

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.

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n/a	Cor	nfirmed
	X	The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement
	X	A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
	X	The statistical test(s) used AND whether they are one- or two-sided Only common tests should be described solely by name; describe more complex techniques in the Methods section.
x		A description of all covariates tested
×		A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons
	X	A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals)
	×	For null hypothesis testing, the test statistic (e.g. <i>F</i> , <i>t</i> , <i>r</i>) with confidence intervals, effect sizes, degrees of freedom and <i>P</i> value noted Give <i>P</i> values as exact values whenever suitable.
x		For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
×		For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
x		Estimates of effect sizes (e.g. Cohen's d , Pearson's r), indicating how they were calculated
		Our web collection on statistics for biologists contains articles on many of the points above

Software and code

Policy information about availability of computer code

Data collection

No commercial, open source or custom code are used to collect the data in this study.

Data analysis

Origin 2023 was used to help finish the plotting and significance analyses, and BD Flowjo 10.8.1 was used to analyzed flow cytometry data in this study. Gaussian 16 program package (revision D. 01) was used to get optimized molecular geometry. AutoDock 4.2 was used to conducted the docking assays. ImageJ 1.52 was used to finished the imagines analyses.

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Portfolio guidelines for submitting code & software for further information.

Data

Policy information about availability of data

All manuscripts must include a <u>data availability statement</u>. This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A description of any restrictions on data availability
- For clinical datasets or third party data, please ensure that the statement adheres to our policy

The authors declare that all data generated or analyzed during this study are available in this published article, supplementary information files and data source file. The full image dataset is available from the corresponding author upon request.

	Research involving h	uman participants,	their data, or	biological material
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Policy information a and sexual orientation		vith human participants or human data. See also policy information about sex, gender (identity/presentation), thnicity and racism.	
Reporting on sex and gender		No human participants or human data is involved in this study.	
Reporting on race, ethnicity, or other socially relevant groupings		No human participants or human data is involved in this study.	
Population character	ristics	No human participants or human data is involved in this study.	
Recruitment		No human participants or human data is involved in this study.	
Ethics oversight		No human participants or human data is involved in this study.	
Note that full informat	Note that full information on the approval of the study protocol must also be provided in the manuscript.		
Field-spe	cific re	porting	
Please select the one	e below that is	the best fit for your research. If you are not sure, read the appropriate sections before making your selection.	
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For a reference copy of th	ne document with a	all sections, see <u>nature.com/documents/nr-reporting-summary-flat.pdf</u>	
Life scien	ces stu	udy design	
All studies must disc	close on these	points even when the disclosure is negative.	
	No sample size calculations were performed. In vitro studies were repeated three times independently with triplicate samples, and in the in vivo experiments with 5 mice were used in each group of the xenograft tumor model and 3 mice were used in each group of in situ hepatocarcinoma model. Statistics such as error bars, significance and p values were derived from n ≥3.		
Data exclusions	No sample size	calculations were performed.	
Replication	All experiments were repeated three times independently and experimental findings were reproducible.		
Randomization	All samples were randomly allocated into experimental groups.		
Blinding	All the investigators were blinded to group allocation in the course of data collection and analysis.		
We require information	n from authors a	Decific materials, systems and methods about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.	
Materials & exp	erimental si	ystems Methods	
n/a Involved in the X Antibodies X Eukaryotic c X Palaeontolo X Animals and Clinical data	e study cell lines gy and archaeol d other organism	n/a Involved in the study ChIP-seq Flow cytometry MRI-based neuroimaging MRI-based neuroimaging neuroimaging MRI-based neuroimaging neuroimagin	
Antibodies			
Antibodies used	(ab927	tibodies for GGT (ab109427, ab55138, rabbit mAb), GPX4 (ab125066, rabbit mAb), β-actin (ab8226, mouse mAb), and Ki67 42, rabbit mAb), goat anti-rabbit IgG H&L (HRP) (ab6721), goat anti-mouse IgG H&L (HRP) (ab205719), and goat anti-rabbit IgG Alexa Fluor® 488 labelled, ab150077) were used and obtained from Abcam.	
Validation	All the	commercial antibodies were validated using Western blotting assays or ELISA assays in preliminary experiment before using	

for this study.

Eukaryotic cell lines

Policy information about cell lines and Sex and Gender in Research

Cell line source(s) HepG2, HeLa and LO2 cells used in this study were obtained from the Cell Bank of the Shanghai Institute of Biochemistry and Cell Biology.

Authentication All the cells authentication were provided by the Cell Bank of the Shanghai Institute of Biochemistry and Cell Biology.

Mycoplasma contamination Mycoplasma screening was conducted routinely, confirming the absence of contamination in all tested cell lines.

Commonly misidentified lines (See <u>ICLAC</u> register)

No of the cell lines used in this study belong to commonly misidentified lines.

Animals and other research organisms

Policy information about <u>studies involving animals</u>; <u>ARRIVE guidelines</u> recommended for reporting animal research, and <u>Sex and Gender in</u> Research

Laboratory animals

4-6 weeks-old female BALB/c nude mice were used in this study.

No wild animals were used in this study.

To eliminate the effect of sex on tumor models, female mice were used in this study. No sex-based reporting was obtained from this study. This study investigated the enhanced photodynamic therapy efficiency of the aggregation-induced emission photosensitizer, so the influence of sex on tumor progression was not taken into account in the design of the study.

Field-collected samples

No filed-collected samples were involved in this study.

All animal experiments were approved by the Institutional Animal Care and Use Committee (IACUC), and all the operations were following the guidelines of the Animal Experiment Center of the Chinese University of Hong Kong (Shenzhen, China, protocol number,

Note that full information on the approval of the study protocol must also be provided in the manuscript.

Plants

Seed stocks No seed stock or plant was used in this study.

Novel plant genotypes No seed stock or plant was used in this study.

CUHKSZ-AE2022004).

Authentication No seed stock or plant was used in this study.

Flow Cytometry

Plots

Confirm that:

- The axis labels state the marker and fluorochrome used (e.g. CD4-FITC).
- The axis scales are clearly visible. Include numbers along axes only for bottom left plot of group (a 'group' is an analysis of identical markers).
- 🗶 All plots are contour plots with outliers or pseudocolor plots.
- 🗶 A numerical value for number of cells or percentage (with statistics) is provided.

Methodology

Sample preparation

For the ROS scavenging experiment, cells were pre-incubated with media containing TBmA-Glu supplemented with ROS scavengers (Trolox: 100 μM, mannitol: 50 mM, Tiron: 10 mM, NaN3: 5 mM) for 12 hours before light irradiation (12 J·cm–2). Afterward, the cells were incubated with basal DMEM medium (without FBS) containing 10 μM DCFH-DA for an additional duration of 20 minutes. The cells were then harvested, centrifuged, washed twice with PBS, resuspended in a volume of PBS (500 μL), and analyzed using flow cytometry. DCF: λex =488 nm, λem =525 nm. A total of 104 cells were collected per sample

and data analysis was performed using FlowJo 10.8.1 software.

Instrument Flow cytometry was conducted on a Beckman Coulter CytoFLEX S (USA).

Software Data analysis was performed using FlowJo 10.8.1 software

Cell population abundance

The cells in each groups were labelled with a ROS indicator DCFH-DA, which could be activated in cell with ROS, resulting the

group.

Gating strategy

In ROS flow cytometry assays, cells and cell fragments are first separated using FSC/SSC signals, which is a standard operation step to ensure that the objects of analysis are intact viable cells. FSC (Forward Scatter) and SSC (Side Scatter) parameters provide information about the size and complexity/granularity of the cells, respectively, helping to distinguish viable cells,

dead cells, debris, and other possible particles.

Next, the signal in the "FITC-channel" of the control groups is analyzed to ensure that the signal intensity is around 2,000. This can achieved by setting a specific voltage or gain to ensure consistency and comparability of the signal throughout the entire experiment. The setting of the FITC channel signal intensity to 2,000 may be based on experimental design and predetermined parameters to facilitate subsequent data analysis and comparison.

generation of a fluorescent DCF. The fluorescence intensity was used to calculated the cell population abundance in each

All tests should then be completed under this condition to ensure the reliability and repeatability of the results, as well as to provide a standardized basis for subsequent data analysis. In this way, the ROS production levels under different samples or conditions can be more accurately assessed and compared.

| X | Tick this box to confirm that a figure exemplifying the gating strategy is provided in the Supplementary Information.