

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](#).

Statistics

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

- | n/a | Confirmed |
|-------------------------------------|--|
| <input type="checkbox"/> | <input checked="" type="checkbox"/> The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> The statistical test(s) used AND whether they are one- or two-sided
<i>Only common tests should be described solely by name; describe more complex techniques in the Methods section.</i> |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> A description of all covariates tested |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons |
| <input type="checkbox"/> | <input checked="" type="checkbox"/> 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) |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> For null hypothesis testing, the test statistic (e.g. F , t , r) with confidence intervals, effect sizes, degrees of freedom and P value noted
<i>Give P values as exact values whenever suitable.</i> |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> 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

The 1H-NMR and 13C-NMR spectra were acquired over Bruker Avance 400 or Avance 600 spectrometers. The ESI-HRMS spectra were obtained using Micromass GCT spectrometer at the Analysis and Testing Center of East China University of Science and Technology. The UV-Vis absorption spectra were acquired using a SHIMADZU UV-2600 UV-VIS spectrophotometer and the fluorescence spectra were acquired with a PTI-QM4 steady-state fluorimeter with 1 cm cuvette and an InGaAs photodetector. The femtosecond transient absorption (fs-TA) spectra were acquired with Helios fire, ultrafast systems. The single crystal X-ray diffraction data were acquired with a Rigaku Synergy-R X-ray single crystal diffractometer. The in vivo fluorescence imaging was carried out with MARS (Artemis Intelligent Imaging) equipped with an InGaAs camera (NIRvana, Teledyne Princeton Instruments). The photoacoustic imaging of solutions and in vivo photoacoustic imaging of mice were performed with the LOIS 3D imaging system (TomoWave Laboratories, USA).

Data analysis

The 1H-NMR and 13C-NMR spectra were processed using MestReNova. The spectral data were processed using Origin 2024b. The microscopy images were analyzed with Image J 1.48. The X-ray crystal diffraction data (cif file) were analyzed using Mercury 3.8, CCDC.

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 [data availability statement](#). 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 spectral data generated in this study have been deposited in the FigShare database under the accession code <https://doi.org/10.6084/m9.figshare.27959742.v1>. Crystallographic data for the structures reported in this Article have been deposited at the Cambridge Crystallographic Data Centre, under deposition numbers CCDC 2120399 (ESI5•Cl-), and 2364282 (ESI5•PF6-). Copies of the data can be obtained free of charge via <https://www.ccdc.cam.ac.uk/structures/>. Requests for additional materials should be addressed to the corresponding author." Atomic coordinates of the optimized computational models of ESI5, ESI5-NS, ESI5-N, ESI5-S, ESI5-C1(-C5) are in Supplementary Data 1.

Research involving human participants, their data, or biological material

Policy information about studies with [human participants or human data](#). See also policy information about [sex, gender \(identity/presentation\), and sexual orientation](#) and [race, ethnicity and racism](#).

Reporting on sex and gender	n/a
Reporting on race, ethnicity, or other socially relevant groupings	n/a
Population characteristics	n/a
Recruitment	n/a
Ethics oversight	n/a

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

Field-specific reporting

Please select the one below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.

Life sciences Behavioural & social sciences Ecological, evolutionary & environmental sciences

For a reference copy of the document with all sections, see [nature.com/documents/nr-reporting-summary-flat.pdf](https://www.nature.com/documents/nr-reporting-summary-flat.pdf)

Life sciences study design

All studies must disclose on these points even when the disclosure is negative.

Sample size	Hela cells seeded on 96 well plates (3000 cells/well, Total 36 well) were counted for CCK8 assay. For animal experiments, We selected sample size based on our previous experience with equivalent experiments, the published literatures. No statistical methods were used to predetermine samples size. The investigators were blinded to group allocation during data collection.
Data exclusions	No data were excluded.
Replication	At least 3 biological replicates were performed for each experiment. All attempts at replication were successful.
Randomization	Samples/organism were allocated into experimental groups randomly.
Blinding	n/a

Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

Materials & experimental systems

n/a	Involvement in the study
<input checked="" type="checkbox"/>	<input type="checkbox"/> Antibodies
<input type="checkbox"/>	<input checked="" type="checkbox"/> Eukaryotic cell lines
<input checked="" type="checkbox"/>	<input type="checkbox"/> Palaeontology and archaeology
<input type="checkbox"/>	<input checked="" type="checkbox"/> Animals and other organisms
<input checked="" type="checkbox"/>	<input type="checkbox"/> Clinical data
<input checked="" type="checkbox"/>	<input type="checkbox"/> Dual use research of concern
<input checked="" type="checkbox"/>	<input type="checkbox"/> Plants

Methods

n/a	Involvement in the study
<input checked="" type="checkbox"/>	<input type="checkbox"/> ChIP-seq
<input checked="" type="checkbox"/>	<input type="checkbox"/> Flow cytometry
<input checked="" type="checkbox"/>	<input type="checkbox"/> MRI-based neuroimaging

Eukaryotic cell lines

Policy information about [cell lines and Sex and Gender in Research](#)

Cell line source(s)	HeLa cells were purchased from Cell Bank of Type Culture Collection of Chinese Academy of Sciences. Sheep red blood cells were purchased from SenBeijia Biological Technology Co., Ltd.
Authentication	None of the cell lines were authenticated.
Mycoplasma contamination	All cell lines tested negative for mycoplasma contamination.
Commonly misidentified lines (See ICLAC register)	No commonly misidentified lines were used in this study.

Animals and other research organisms

Policy information about [studies involving animals; ARRIVE guidelines](#) recommended for reporting animal research, and [Sex and Gender in Research](#)

Laboratory animals	Six to eight-week-old female BALB/c mice purchased from Shanghai JieSiJie Laboratory Animals were used. The mice were housed in an environment with a temperature of ~25 °C and a 12h light/dark cycle, suitable humidity (typically 40%-60%).
Wild animals	The study did not involve wild animals.
Reporting on sex	Female BALB/c mice were used for in vivo imaging. Sex was not noted in the mouse imaging studies because the results are applicable to both male and female mice.
Field-collected samples	n/a
Ethics oversight	The animal experiment protocol was approved by the Laboratory Animal Welfare and Ethics Committee of Shanghai University of Traditional Chinese Medicine (PZSHUTCM220613018, June 13, 2022).

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

Plants

Seed stocks	n/a
Novel plant genotypes	n/a
Authentication	n/a