

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

- | | | |
|-------------------------------------|-------------------------------------|--|
| ☐ | ☒ | The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement |
| ☐ | ☒ | A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly |
| ☐ | ☒ | 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> |
| ☒ | ☐ | A description of all covariates tested |
| ☒ | ☐ | A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons |
| ☐ | ☒ | 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. 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> |
| ☒ | ☐ | 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 |
| ☐ | ☒ | 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

Bruker AVANCE NEO 500 NMR spectrometer, PerkinElmer LAMBDA 365 spectro-photometer, BRUKER DALTONICS Matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF-MS), Edinburgh FLS1000 luminescence spectrometer, Laser Particle Size Zeta Potentiometer (Bruker-haven), Talos L120C transmission electron microscope (TEM), The 660 nm fiber-coupled laser and fiber jumper (Changchun Femto-second Technology Co., Ltd.), Confocal laser scanning microscopy (CLSM) images (ZEISS-LSM880 CLSM) , γ -counter (2480 Wizard2, PerkinElmer, USA), Super Nova[®] PET/CT system, in vivo imaging system (IVIS) Spectrum, Hematoxylin and Eosin (H&E) staining (Servicebio Technology Co., Ltd. (Wu-han, China)), blood chemistry and blood routine (Vital River Laboratory Animal Technology Co., Ltd. (Beijing, China)), hematoxylin-eosin (H&E) staining, reactive oxygen species (ROS) staining, terminal deoxynucleotidyl transferase deoxyuridine triphosphate (dUTP) nick end labeling (TUNEL) assay and Ki67 im-munohistochemical staining of sections of the T24 tumor tissue (Wuhan Servicebio Technology Co., Ltd.).

Data analysis

Bar graph, curves and the relevant statistics were analyzed by GraphPad Prism8.0 and origin 9.0; Confocal data were analyzed by ZEISS ZEN Microscopy Software; All the calculations were performed with C.01 revision of the Gaussian 16 program using the B3LYP functional and 6-311G(d,p) basis set. The frequency calculation was also carried out on all optimized geometries to confirm that no imaginary frequencies were obtained. The spin-orbital coupling (SOC) matrix element values of compound were calculated using pysoc program package. Molecular dynamics (MD) simulations were conducted utilizing the GROMACS (2023.3) software package, employing the amber03 force field. The restrained electrostatic potential (RESP) fitting technique was applied to derive partial charges for each molecule.

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](#)

All the data generated in this study are provided in the Supplementary Information/Source Data file.

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

Reporting on race, ethnicity, or other socially relevant groupings

Population characteristics

Recruitment

Ethics oversight

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

Data exclusions

Replication

Randomization

Blinding

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	Involved in the study
☒	☐ Antibodies
☐	☒ Eukaryotic cell lines
☒	☐ Palaeontology and archaeology
☐	☒ Animals and other organisms
☒	☐ Clinical data
☒	☐ Dual use research of concern
☒	☐ Plants

Methods

n/a	Involved in the study
☒	☐ ChIP-seq
☐	☒ Flow cytometry
☒	☐ MRI-based neuroimaging

Eukaryotic cell lines

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

Cell line source(s)	T24, U-87MG, L929 and HeLa cell line were purchased from the Cell Culture Center of the Institute of Basic Medicine, Chinese Academy of Medical Sciences (Beijing, China).
Authentication	None of the cell lines used were authenticated.
Mycoplasma contamination	All the cells were cultured for less than 3 months, and tested for mycoplasma contamination.
Commonly misidentified lines (See ICLAC register)	No commonly misidentified cell lines was 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	Female BALB/c nude mice (~8 weeks old, 18 g) were purchased from Vital River Laboratory Animal Technology Co., Ltd. (Beijing, China).
Wild animals	The study did not involve wild animals.
Reporting on sex	Sex and gender of BALB/c nude mice has been collected and recorded by authors, which has no bearing on data analysis or results.
Field-collected samples	The study did not involve samples collected from the field.
Ethics oversight	All animal experiments were approved by the Committee for Animal Research of the Harbin Medical University (HMUIRB2025063PRE)

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

Plants

Seed stocks	Not used
Novel plant genotypes	Not used
Authentication	Not used

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	The sample preparation was described in the methods section
Instrument	NovoCyte 451190832384
Software	NovoExpress 1.5.0
Cell population abundance	In each analysis, minimum of 5000 cells were counted.
Gating strategy	The gating strategy were shown in the Supplementary Figure 9.

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