

# RSC Medicinal Chemistry

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## IN THIS ISSUE

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### Cover

See Kevin A. Scott *et al.*, pp. 743–767.

Image reproduced by permission of Kevin Scott from *RSC Med. Chem.*, 2026, 17, 743.

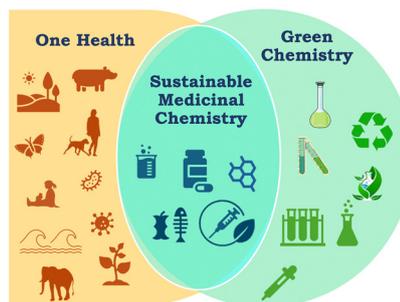
Bottle of cantharidin photographed at the Museum of Pharmacy, University of Arizona, by Kris Hanning. Blister beetle photograph permissions from Shutterstock. Protein complex of PPP2CA/PPP2R1A/PPP2R2A modelled using AlphaFold3, PyMol, and Schrödinger Maestro by KAS.

## OPINION

738

### The many facets of sustainability in medicinal chemistry: our personal experience

Bianca Martinengo, Eleonora Diamanti, Elisa Uliassi and Maria Laura Bolognesi\*

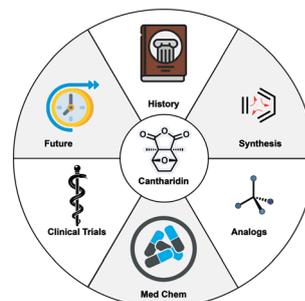


## REVIEWS

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### On the history, synthesis, and medicinal use of cantharidin, LB-100, and their analogs

Kevin A. Scott,\* Adam McCluskey, Jon T. Njardarson and Wei Wang





# RSC Advances

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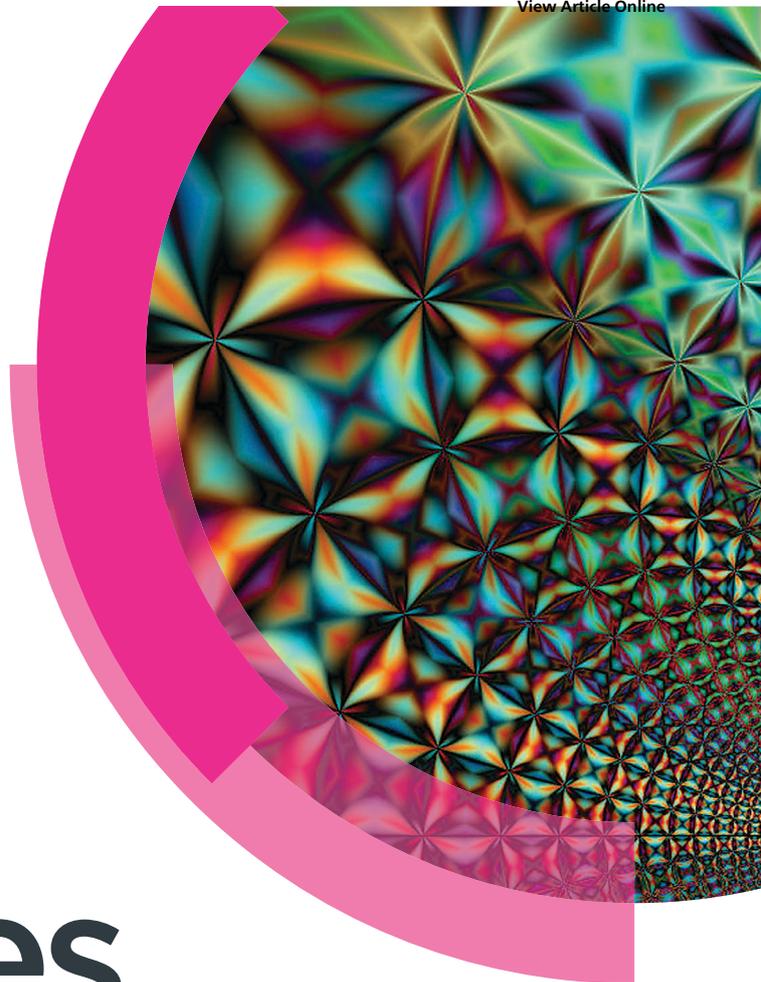


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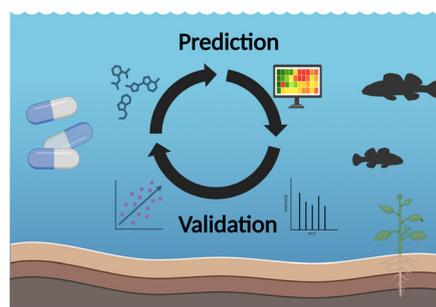


## REVIEWS

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## From lab to environment: forecasting pharmaceutical impact using *in silico* and analytical tools

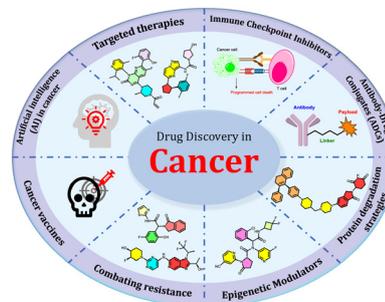
Hamza Boucetta, Peije Russell, David Rudd\* and Manuela Jörg\*



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## An overview of recent advancements in targeted cancer therapies and their potential clinical impact

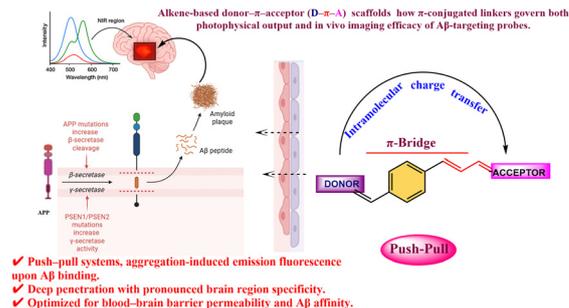
Shujauddin Ahmed, Akash P. Sakla, Kousar Jahan, Naziya Neshat, Mymoona Akhter, Shams Aghaz\* and Ahmed Kamal\*



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## Theranostic advances in Alzheimer's disease: structure-guided design of near-infrared fluorescent probes targeting amyloid- $\beta$ and cholinergic dysfunction

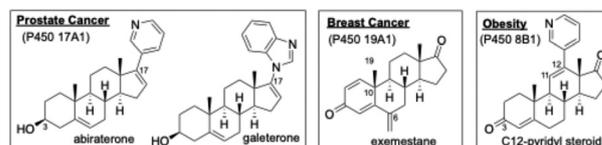
Upesh Mandloi, Namita Giri, Saroj Kumar and Gyan Modi\*



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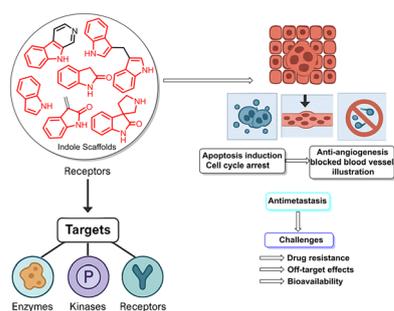
## Strategies to inhibit steroid cytochrome P450 enzymes to benefit human health: development of steroid ligands for P450s 17A1, 19A1, and 8B1 to treat cancer and obesity

Tu M. Ho and Francis K. Yoshimoto\*



## REVIEWS

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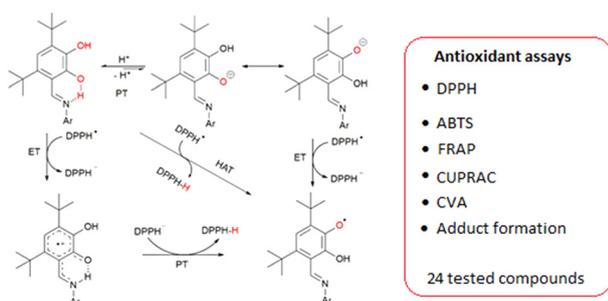


## Recent developments in the discovery of indole-based scaffolds as promising targeted cancer therapeutics

Prasanna A. Yakkala, Venkatesh Erram, Sajeli A. Begum and Ahmed Kamal\*

## RESEARCH ARTICLES

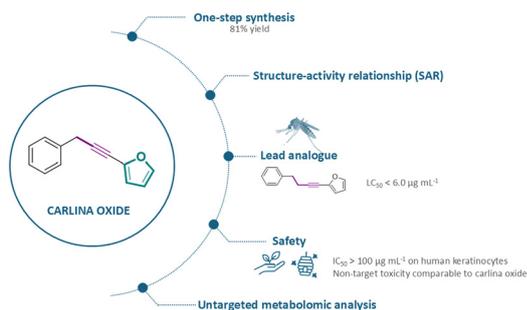
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## Sterically hindered catechol-derived Schiff bases: design, synthesis, SAR analysis and mechanisms of the antioxidant activity

Maxim Gvozdev, Iveta Turomsha, Nikolai Osipovich, Roman Sverdlov and Natalia Loginova\*

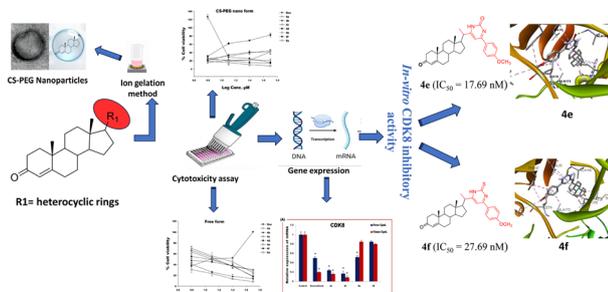
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## Harnessing carlina oxide scaffold for the management of vector-borne diseases: synthesis and structure-activity relationship

Eleonora Spinozzi,\* Alessia Piergentili, Marta Ferrati, Cecilia Baldassarri, Giada Trebaiocchi, Paolo Rossi, Fabrizio Araniti, Alice Zambelli, Loredana Cappellacci, Laura Zeppa, Martina Giangrossi, Alessandro Palmieri, Roman Pavela, Filippo Maggi and Riccardo Petrelli

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## Discovery of novel progesterone-heterocyclic conjugates and their encapsulated polymeric nanoparticles as potential CDK8 inhibitors: lung cytotoxicity evaluation, gene expression, and molecular docking

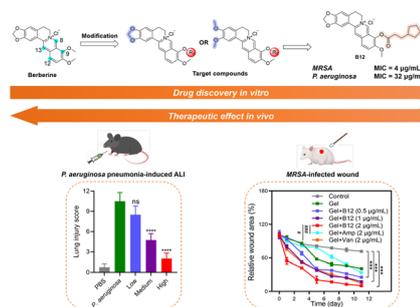
Yasmin Y. Omar, Ghada F. Elmasry,\* Dina S. El-kady, Ahmed A. Abd-Rabou, Samir M. El-Moghazy, Fadi M. Awadallah, Gamal A. Elmegeed and Ghada H. Elsayed\*



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## Synthesis, antibacterial activity, and mechanistic characterization of novel 9-substituted berberine derivatives

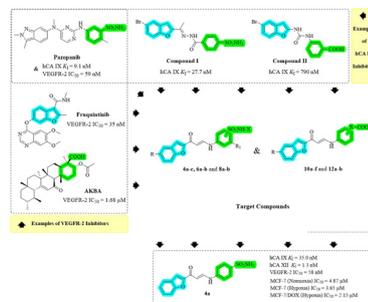
Jiaying Tong, Huamao Yang, Yeying He, Kejie Chen, Chaoyue Chen, Haoyi Han and Chenping Li\*



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## Discovery of enamione-linked benzofuran derivatives as dual VEGFR-2/hCA IX inhibitors exhibiting hypoxia-mediated chemosensitization

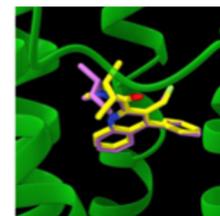
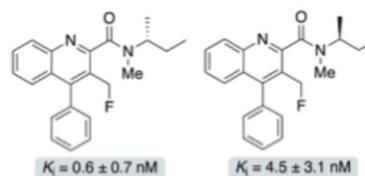
Wagdy M. Eldehna,\* Zainab M. Elsayed, Mohamed R. Elnagar, Andrea Ammara, Mahmoud S. Elkotamy, Rehan Monir, Alessio Nocentini, Mohammed M. Al-Sanea, Claudiu T. Supuran, Haytham O. Tawfik,\* Hatem A. Abdel-Aziz and Ahmed T. Negrmedin



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## Synthesis and evaluation of enantiomeric quinoline-2-carboxamides: positron emission tomography imaging agents for the translocator protein

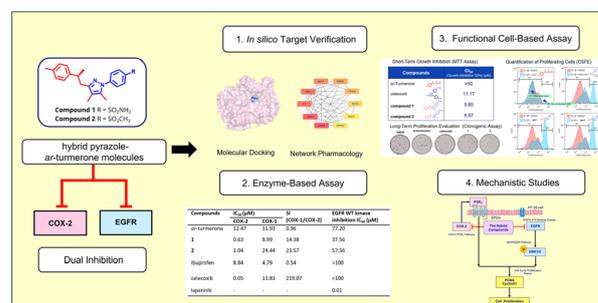
Lachlan J. N. Waddell, Mark G. MacAskill, Holly McErlain, Timaeus E. F. Morgan, Lewis Williams, Victoria J. M. Reid, Anna Beyger, Sally L. Pimlott, Adriana A. S. Tavares and Andrew Sutherland\*



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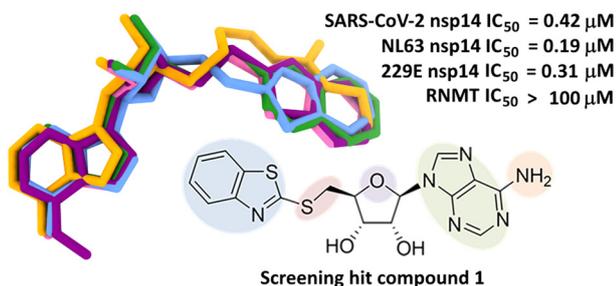
## Dual COX-2 and EGFR inhibition by pyrazole-*ar*-turmerone hybrids suppresses colorectal cancer cell proliferation

Monsin Sangsawat, Nonthaneth Nalinratana, Waraluck Chaichompoo, Opa Vajragupta, Hua Zhu, Yilin Song, Worathat Thitikornpong\* and Pornchai Rojsitthisak



## RESEARCH ARTICLES

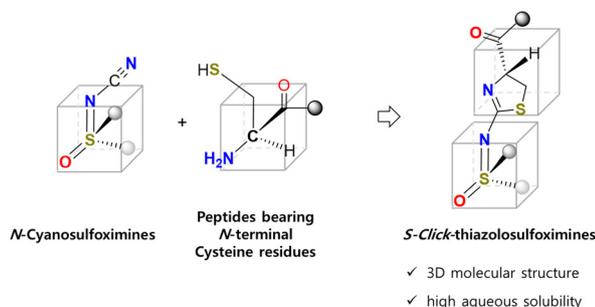
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### Crystallographic characterisation and development of bi-substrate inhibitors of coronavirus nsp14 methyltransferase

I. Georgiou, C. Robinson, S. N. O'Byrne, A. Matsuda, P. Grygier, C. D. Smith, S. O'Neill, S. A. Ahmad, S. Norval, J. M. Post, M. Groenewold, N. Urakova, P. Wanningen, L. Kresik, J. Plewka, A. Delpal, K. See, T. Eadsforth, K. Wierzbicka, E. Decroly, K. S. Saikatendu, E. Chang, E. J. Snijder, K. Pyrc, A. Czarna,\* D. E. Scott\* and I. H. Gilbert\*

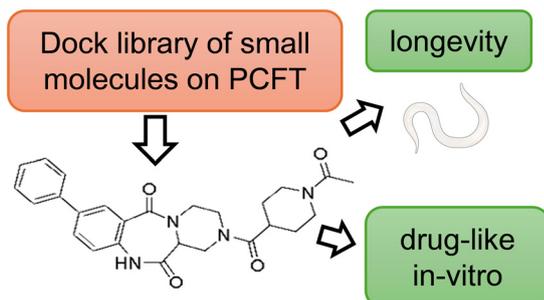
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### *N*-Cyano sulfoximine-mediated thiazole ligation with *N*-terminal cysteine under mild aqueous conditions

Eunsil Kim, Ji Young Hyun, Ji Ho Song, Hwan Jung Lim\* and Seong Jun Park\*

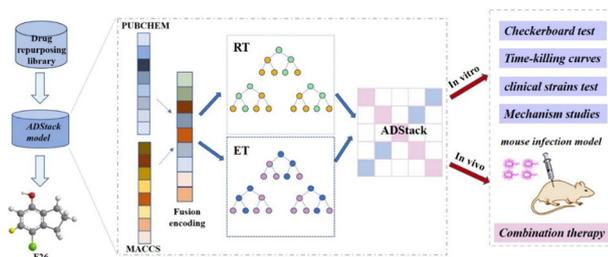
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### A new compound that extends the lifespan of worms, with favorable *in vitro* properties and a lack of toxicity in rodents

Heidi M. Blank and Michael Polymenis\*

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### Discovery of novel polymyxin E adjuvants against *Acinetobacter baumannii* guided by a stacking-based machine learning model

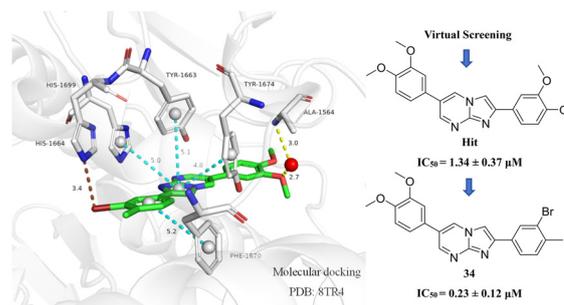
Yuce Chen, Kunkun Shen, Ting Lin, Daijie Chen, Zhong Li, Yuheng Yang\* and Xiaoyong Xu\*



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### Novel pyrimido[1,2-*a*]imidazole derivatives as potent Pks13-TE inhibitors: structure-based virtual screening and rational design

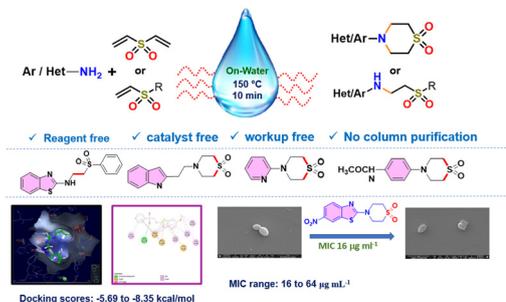
Xiangying Li, Yuanyuan Liu, Wen Shao, Deling Jiang, Xupeng Huang,\* Zihe Rao,\* Wei Peng\* and Yuying Fang\*



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### Microwave-assisted single-step synthesis of cyclic and acyclic $\beta$ -aminosulfones and evaluation of their antifungal activity targeting CYP51

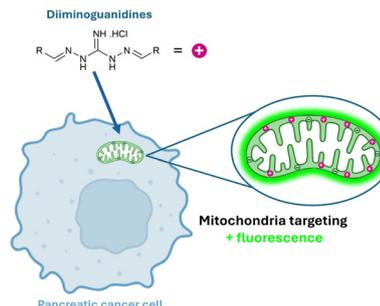
Abigail Bibiana Pinheiro, Soumik Saha, Madhuri Madduri, Utpal Roy, Lakshmi Sudhir Menon, Sumit Biswas, Amrita Chatterjee\* and Mainak Banerjee\*



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### Mitochondria-targeting symmetric diiminoguanidines: potent and selective anticancer agents against pancreatic tumors

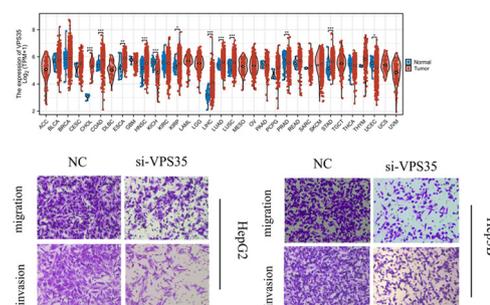
Sigrid Lacaille\* and Andreea R. Schmitzer\*



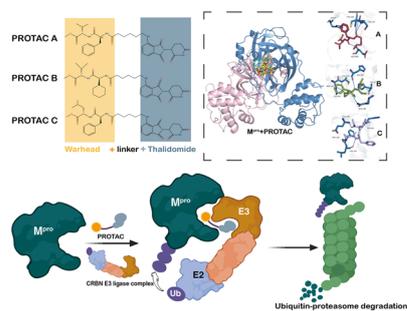
1107

### Comprehensive multi-omics analysis and experimental validation indicate that VPS35 is a promising biomarker for prognosis, immunotherapy, and chemotherapy in LIHC

Dan Wan, Yajie Qi, Yali Kang, Fanfan Liang, Qian Wang, Hailong Zhang, Shaoying Zhang and Xiao Liang\*



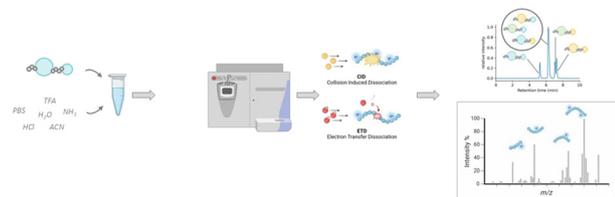
1135



### Integrated computational screen and validation of thalidomide-based PROTACs targeting SARS-CoV-2 main protease

Li-Na Guo, Yu-Hua Li, Rou-Yu Zhu, Ni Su, Zhi-Yu Shao\* and Hua Diao\*

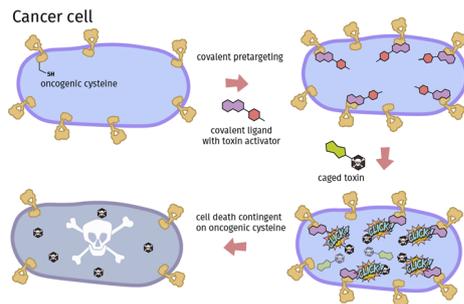
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### Revealing deamidation and isoaspartate formation during peptide analysis, purification and storage by tandem mass spectrometry

V. Erckes, L. Chamera Rendueles, A. Misiek and C. Steuer\*

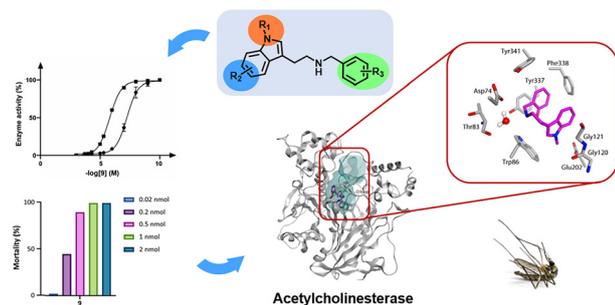
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### Exploiting intracellular oncogenic proteins to release cytotoxins

Matthias Schild and Dennis Gillingham\*

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### Potent and selective indole-based inhibitors targeting disease-transmitting mosquitoes

R. Rajeshwari, V. Duvauchelle, C. Lindgren, K. Stangner, S. Knutsson, N. Forsgren, F. Ekström, L. Kamau and A. Linusson\*

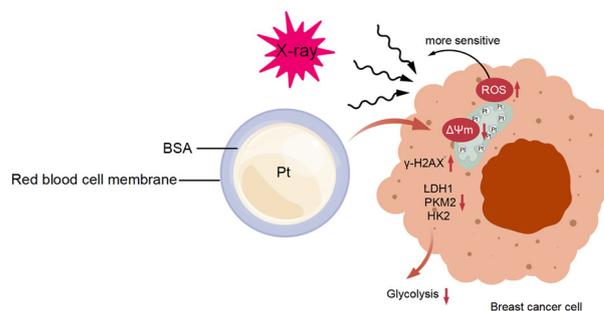


## RESEARCH ARTICLES

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### Novel Pt@BSA nanoparticles improve radiotherapeutic outcomes in breast cancer

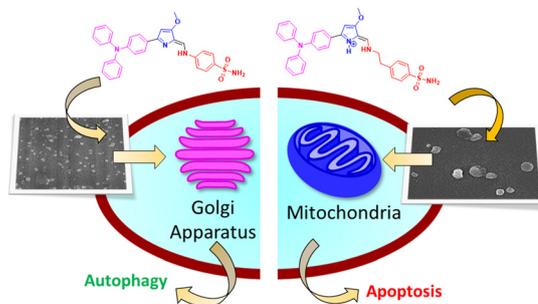
Yuhui Zhang,\* Yihui Liu and Dongju Zheng



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### Small molecule-mediated spatial targeting of mitochondria and the Golgi apparatus in cancer cells

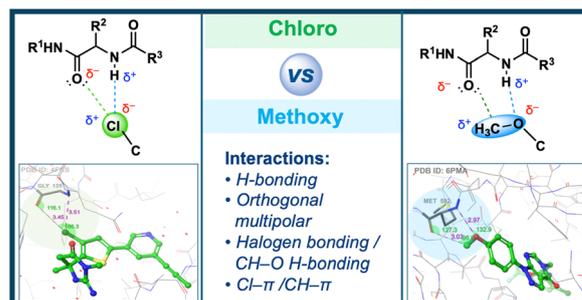
Phanindra Kumar, Asima Sahu, Tripti Mishra and Sudipta Basu\*



1207

### Parallels between the chloro and methoxy groups for potency optimization

Debora Chiodi and Yoshihiro Ishihara\*



## CORRECTION

1231

### Correction: Design, synthesis, and anti-plasmodial profiling of oxalamide-linked 4-aminoquinoline-phthalimide hybrids

Nikita Gupta, Anu Rani, Kewal Kumar, Raghu Raj\* and Vipin Kumar\*

