

## Yao Xiao Jun



Position : Professor

Faculty: Dr. Neher's Biophysics Laboratory for  
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### Research Areas:

Computer-aided drug design, bioinformatics and computational biology, chemoinformatics and chemometrics.

### Education:

1998.7 B.Sc. in Chemistry, Lanzhou University

2003.7 Ph.D. in Analytical Chemistry, Lanzhou University

2004.12 Ph. D. in Chemoinformatics and Theoretical Chemistry, University Paris 7-Denis  
Diderot, France

### Working Experience:

2005.1- Professor, College of Chemistry and Chemical Engineering, Lanzhou University

2013.9- Professor, Macau Institute for Applied Research in Medicine and Health, State Key  
Laboratory for Quality Research in Chinese Medicines Macau University of Science and  
Technology

### Publications:

1. Zhang J, Zhang J, Liu Q, Fan XX, Leung EL\*, Yao XJ\*, Liu L\*. Resistance looms for KRAS G12C inhibitors and rational tackling strategies. *Pharmacol Ther.* 2021, 229:108050.
2. Liu Q, Wang Y, Leung EL, Yao X\*. In silico study of intrinsic dynamics of full-length apo-ACE2 and RBD-ACE2 complex. *Comput Struct Biotechnol J.* 2021, 19:5455-5465.

3. Wang Q, Shao X, Leung ELH, Chen Y, Yao X. Selectively targeting individual bromodomain: Drug discovery and molecular mechanisms. *Pharmacol Res.* 2021, 172:105804.
4. Jiang ZB, Wang WJ, Xu C, Xie YJ, Wang XR, Zhang YZ, Huang JM, Huang M, Xie C, Liu P, Fan XX, Ma YP, Yan PY, Liu L, Yao XJ\*, Wu QB\*, Leung EL\*. Luteolin and its derivative apigenin suppress the inducible PD-L1 expression to improve anti-tumor immunity in KRAS-mutant lung cancer. *Cancer Lett.* 2021, 515:36-48.
5. Liang TL, Li RZ, Mai CT, Guan XX, Li JX, Wang XR, Ma LR, Zhang FY, Wang J, He F, Pan HD, Zhou H, Yan PY, Fan XX, Wu QB, Neher E, Liu L, Xie Y\*, Leung EL\*, Yao XJ\*. A method establishment and comparison of in vivo lung cancer model development platforms for evaluation of tumour metabolism and pharmaceutical efficacy. *Phytomedicine.* 2021, 5:153831.
6. Lai HL, Fan XX, Li RZ, Wang YW, Zhang J, Liu L, Neher E\*, Yao XJ\*, Leung EL\*. Roles of Ion Fluxes, Metabolism, and Redox Balance in Cancer Therapy. *Antioxid Redox Signal.* 2021, 34:1108-1127.
7. Osama A, Zhang J, Yao J, Yao X\*, Fang J\*. Nrf2: a dark horse in Alzheimer's disease treatment. *Ageing Res Rev.* 2020, 64:101206.
8. Wang WJ, Mao LF, Lai HL, Wang YW, Jiang ZB, Li W, Huang JM, Xie YJ, Xu C, Liu P, Li YM\*, Leung ELH\*, Yao XJ\*. Dolutegravir derivative inhibits proliferation and induces apoptosis of non-small cell lung cancer cells via calcium signaling pathway. *Pharmacol Res.* 2020, 161:105129.
9. Leung EL, Luo LX, Li Y, Liu ZQ, Li LL, Shi DF, Xie Y, Huang M, Lu LL, Duan FG, Huang JM, Fan XX, Yuan ZW, Ding J, Yao XJ\*, Ward DC\*, Liu L\* Identification of a new inhibitor of KRAS-PDE $\delta$  interaction targeting KRAS mutant nonsmall cell lung cancer. *Int J Cancer.* 2019, 145:1334-1345.
10. Leung ELH, Luo LX, Liu ZQ, Wong VKW, Lu LL, Xie Y, Zhang N, Qu YQ, Fan XX, Li Y, Huang M, Xiao DK, Huang J, Zhou YL, He JX, Ding J, Yao XJ\*, Ward DC\*, Liu L\*. Inhibition of KRAS-dependent lung cancer cell growth by deltarasin: blockage of autophagy increases its cytotoxicity. *Cell Death Dis.* 2018, 9:216.