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Title: ^{11}C Labeled Pictilisib (GDC-0941) as a Molecular Tracer Targeting Phosphatidylinositol 3-kinase (PI3K) for Breast Cancer Imaging

Authors: Na Han,^{1,2,3} Yaquin Jiang,^{1,2} Yongkang Gai,^{1,2} Qingyao Liu,^{1,2} Lujie Yuan,^{1,2} Yichun Wang,^{1,2} Mengting Li,^{1,2} Yongxue Zhang,^{1,2} Xiaoli Lan,^{1,2*}

Author information

¹*Department of Nuclear Medicine, Union Hospital, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430022, China*

²*Hubei Key Laboratory of Molecular Imaging, Wuhan 430022, China*

³*Department of Nuclear Medicine, The Affiliated Hospital of Qingdao University, No.16 JiangSu Road, Qingdao, Shandong Province 266000, China*

***Corresponding author:** Xiaoli Lan, M.D, Ph.D.

Address: Department of Nuclear Medicine, Union Hospital, No. 1277 Jiefang Ave, Wuhan, Hubei Province 430022, China.

Tel.: +86-27-83692633(O), +86-13886193262(mobile); Fax: +86-27-85726282.

E-mail: LXL730724@hotmail.com

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Conflicts of interest

The authors declare no potential conflicts of interest.

Supplement data

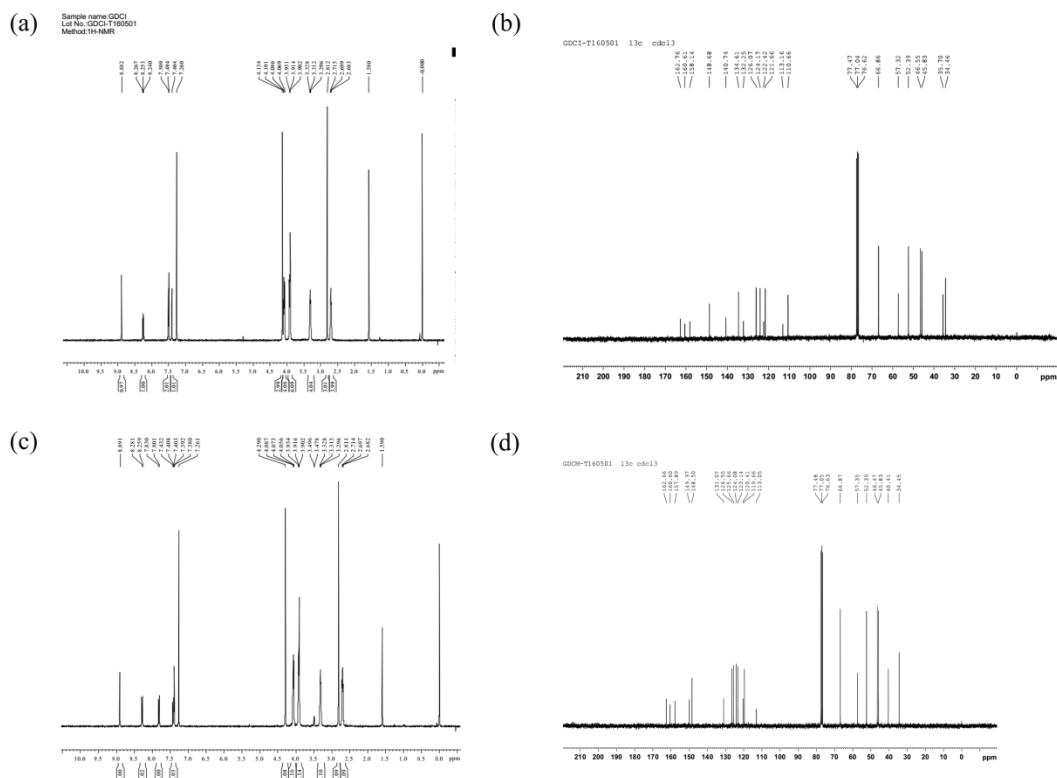


Figure S1: (a) and (b) showed the $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ of GDCI. (c) and (d) showed the $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ of GDCM.

NMR spectroscopy:

GDCI $^1\text{H-NMR}$ (300MHz, CDCl_3) :

δ 8.882(s,1H), δ 8.253(t, $J=4.05\text{Hz}$,1H), δ 7.494(d, $J=4.5\text{Hz}$,2H), δ 7.404(s,1H), δ 4.134(s,3H), δ 4.086(t, $J=4.8\text{Hz}$,4H), δ 3.914(t, $J=5.1\text{Hz}$,4H), δ 3.902(s,2H), δ 3.312(t, $J=4.8\text{Hz}$,4H), δ 2.812(s,3H), δ 2.699(t, $J=4.8\text{Hz}$,4H);

GDCI $^{13}\text{C NMR}$ (CDCl_3):

δ 162.76,160.61,158.14,148.68,140.74,134.61,132.25,126.07,124.17,122.42,121.66,113.16,110.66,77.47,77.04,76.62,66.86,57.32,52.39,46.55,45.83,35.70,34.46;

GDCM $^1\text{H-NMR}$ (300MHz, CDCl_3):

δ 8.891(s,1H), δ 8.259(d, $J=6.6\text{Hz}$,1H), δ 7.801(d, $J=8.7\text{Hz}$,1H), δ 7.408(dd, $J=7.2,8.7\text{Hz}$,1H), δ 7.380(s,1H), δ 4.290(s,3H), δ 4.073(t, $J=4.65\text{Hz}$,4H), δ 3.916(t, $J=4.8\text{Hz}$,4H), δ 3.902(s,2H), δ 3.313(t, $J=4.8\text{Hz}$,4H), δ 2.811(s,3H), δ 2.697(t, $J=4.8\text{Hz}$,4H);

GDCM ¹³CNMR(CDCl₃):

δ162.66,160.60,157.89,149.97,148.50,131.07,126.55,125.66,124.08,123.14,120.41,119.66,113.05,77.48,77.05,76.63,66.87,57.35,52.39,46.47,45.83,40.41,34.45.

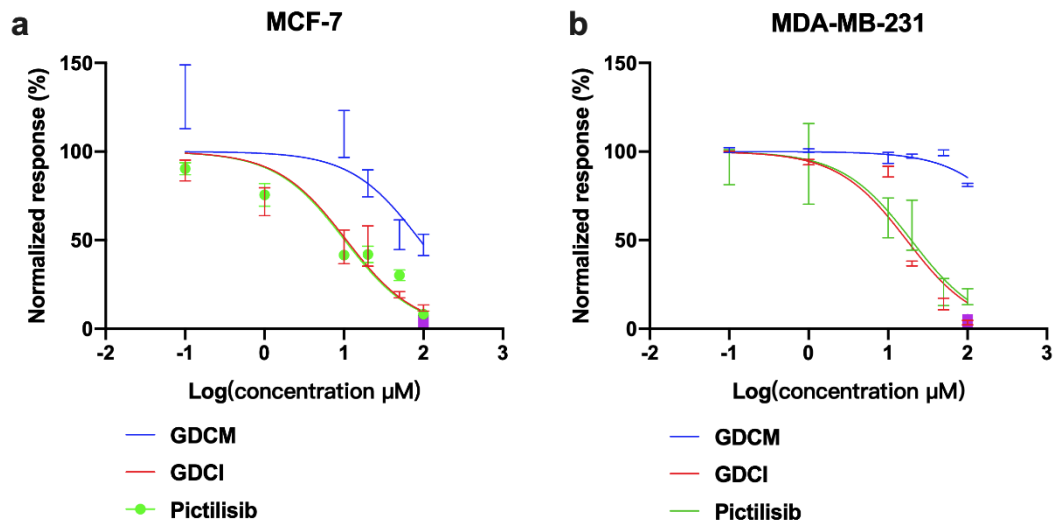


Figure S2 Normalized dose response of the drug for the two cell lines

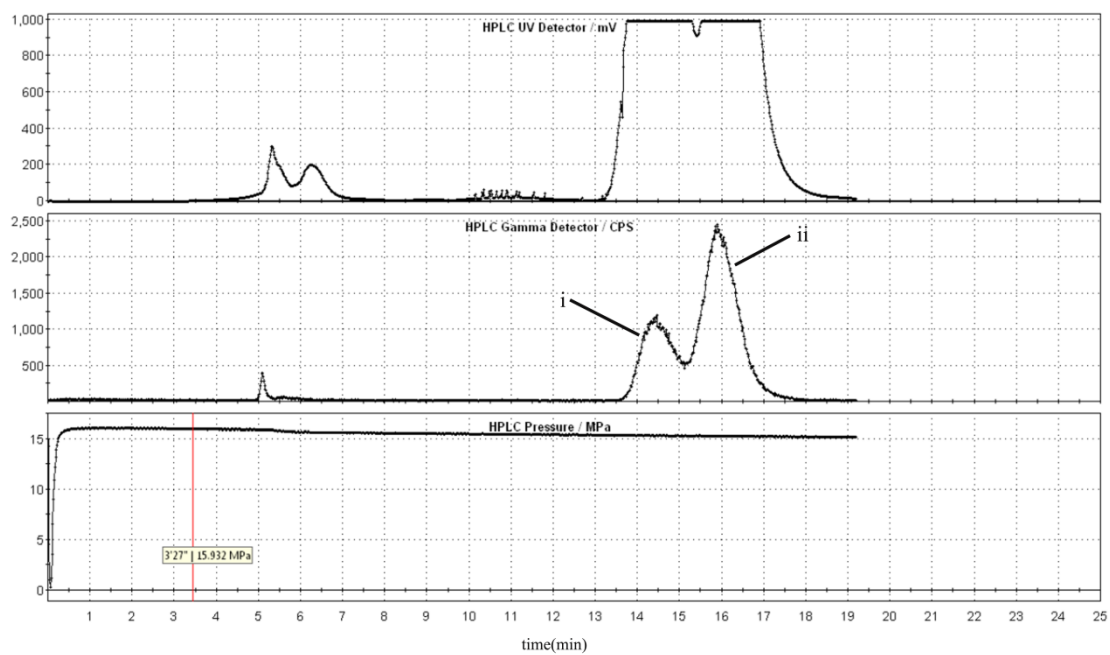


Figure S3: The reaction products were purified by semi-preparative HPLC. i was [^{11}C]-GDCM and ii was [^{11}C]-GDCl.