

Supporting Information

Drug Screening for Glycolysis Pathway in Living Cancer Cells Using ^{19}F

NMR

Biao Liu ^a, Tao Huang ^a, Xiong Xiao ^{a, b}, Xin Chai ^a, Yating Lei ^{a, b}, Qiuyun Sun ^a, Qin Hu ^{a, b}, Qinjun Zhu ^a, Danyun Zeng ^{a, b}, Caixiang Liu ^{a, b}, Lichun He ^{a, b}, Zhou Gong ^{a, b}, Bin Jiang ^{a, b, c}, Xin Zhou ^{a, b, c}, Maili Liu ^{a, b, c, *}, Xu Zhang ^{a, b, c, *}

^a Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology, State Key Laboratory of Magnetic Resonance Spectroscopy and Imaging, National Center for Magnetic Resonance in Wuhan, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement of Science and Technology, Chinese Academy of Sciences, Wuhan, 430071, China.

^b University of Chinese Academy of Sciences, Beijing, 100049, China.

^c Optics Valley Laboratory, Wuhan, 430074, China.

* To whom correspondence should be addressed.

E-mail: ml.liu@apm.ac.cn (Maili Liu); zhangxu@apm.ac.cn (Xu Zhang)

Table of Content

Figure S1. ^{19}F -NMR spectra of supernatant (a) and cell lysate (b) obtained from cell samples after completion of the real-time NMR experiment.	S3
Figure S2. ^{19}F NMR spectra of 0.5 mM BAY-876 in DMSO-d6.....	S3
Figure S3. Normalized LDH concentrations in the bioreactor, measured at the start and end of the experiment, together with the normalized LDH concentrations in the cell lysate (2×10^7 MCF-7 cells).	S4
Figure S4. Cell viability of MCF-7 cells treated with 0.8 mg/ml TCM for 5 h, as measured by CCK-8 assay.	S4
Figure S5. Images of MCF-7 cells before (a) and after (b) NMR experiment stained with trypan blue. (c) Cell viability of MCF-7 cells after the NMR experiment, determined by trypan blue assay.....	S5
Table S1. Chemical shifts of 2-FDG metabolites from ^{19}F spectra.	S6

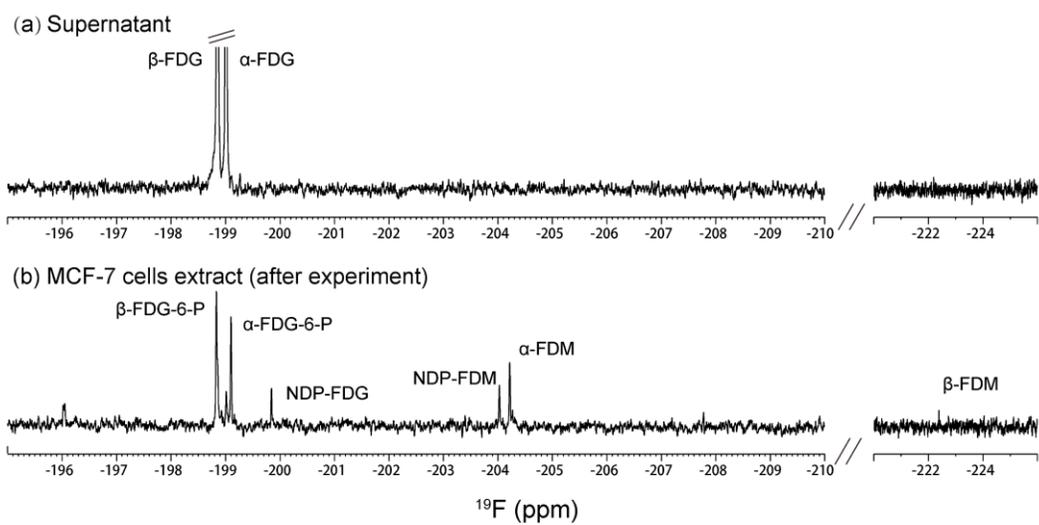


Figure S1. ^{19}F -NMR spectra of supernatant (a) and cell lysate (b) obtained from cell samples after completion of the real-time NMR experiment.

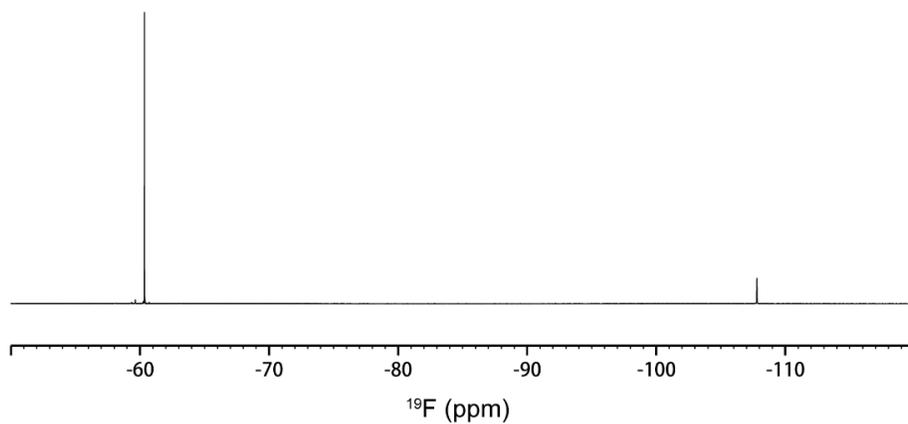


Figure S2. ^{19}F NMR spectra of 0.5 mM BAY-876 in DMSO-d_6 .

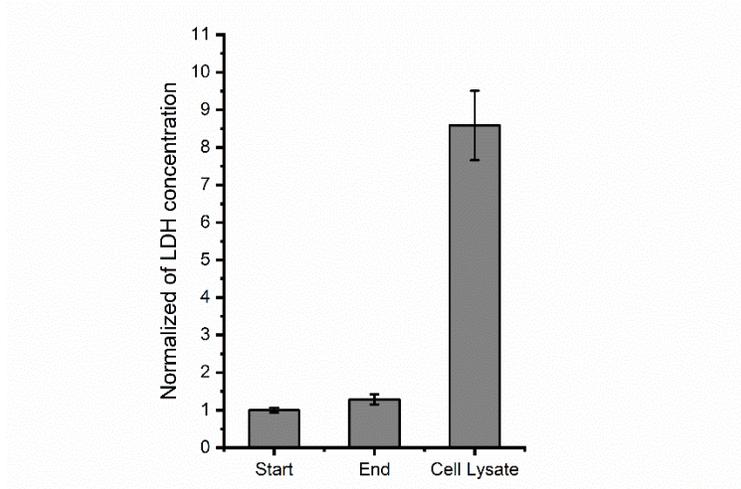


Figure S3. Normalized LDH concentrations in the bioreactor, measured at the start and end of the experiment, together with the normalized LDH concentrations in the cell lysate (2×10^7 MCF-7 cells).

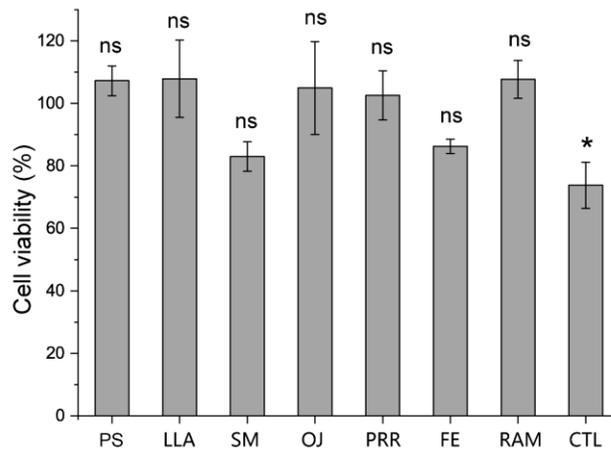


Figure S4. Cell viability of MCF-7 cells treated with 0.8 mg/ml TCM for 5 h, as measured by CCK-8 assay.

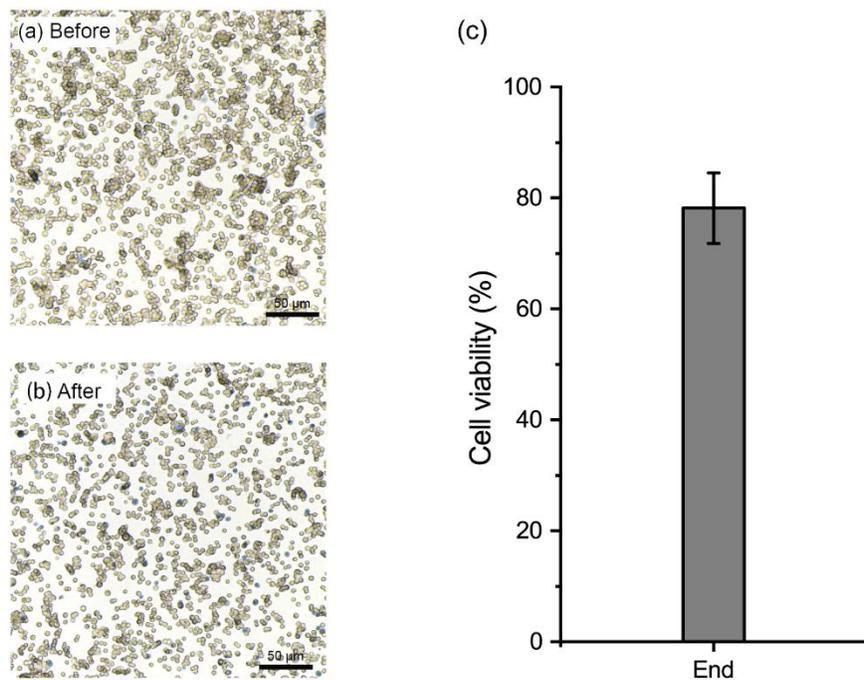


Figure S5. Images of MCF-7 cells before (a) and after (b) NMR experiment stained with trypan blue. (c) Cell viability of MCF-7 cells after the NMR experiment, determined by trypan blue assay.

Table S1. Chemical shifts of 2-FDG metabolites from ^{19}F spectra.

2-FDG metabolites	Chemical shift (ppm)
2-FD-6-PGL	-196.036
β -FDG-6-P	-198.851
β -FDG	-198.852
α -FDG	-199.011
α -FDG-1-P	-199.007
α -FDG-6-P	-199.106
NDP-FDG	-199.836
α -FDM-6-P	-204.155
NDP-FDM	-204.212
α -FDM	-204.264
β -FDM-6-P	-222.503
β -FDM	-222.781