

Supporting information

Structural optimization of icaritin for advanced cancer: novel carbamates via oral administration

Authors:

Fengxiao Li¹, Weiping Wang¹, Jiaqi Fan¹, Yixiu Zhai¹, Jiaming Zhang¹, Tianhong Zhang^{1*}, Qikun Jiang^{1,2*}

Affiliation:

¹ Wuya College of Innovation, Shenyang Pharmaceutical University, Shenyang 110016, PR China;

² State Key Laboratory of Natural and Biomimetic Drugs, Peking University, Beijing 100871, China.

*Correspondence:

Prof. Tianhong Zhang and Prof. Qikun Jiang

No. 120 Mailbox, School of Pharmacy, Shenyang Pharmaceutical University, 103 Wenhua Road, Shenyang 110016, China.

Tel/Fax: +86-24-23984159; +86-24-23986321

E-mail:

zhangth1058@aliyun.com

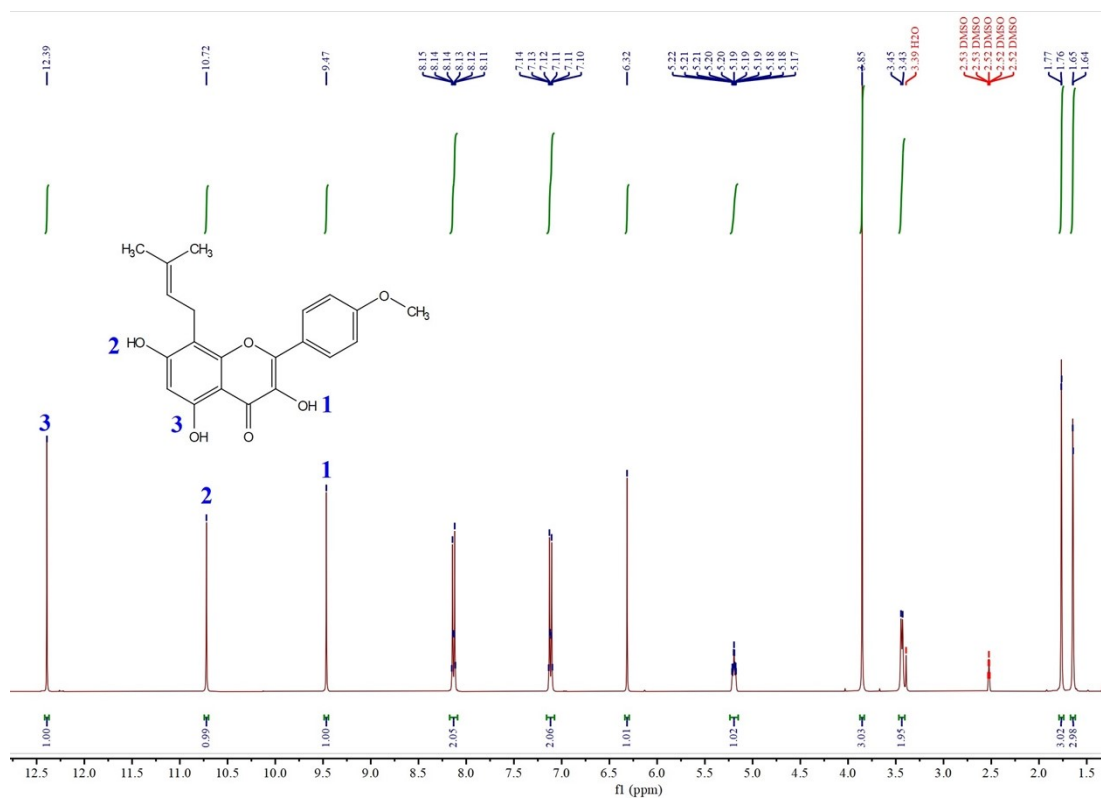


Figure S1. $^1\text{H-NMR}$ ($\text{DMSO-}d_6$) chart of icaritin.

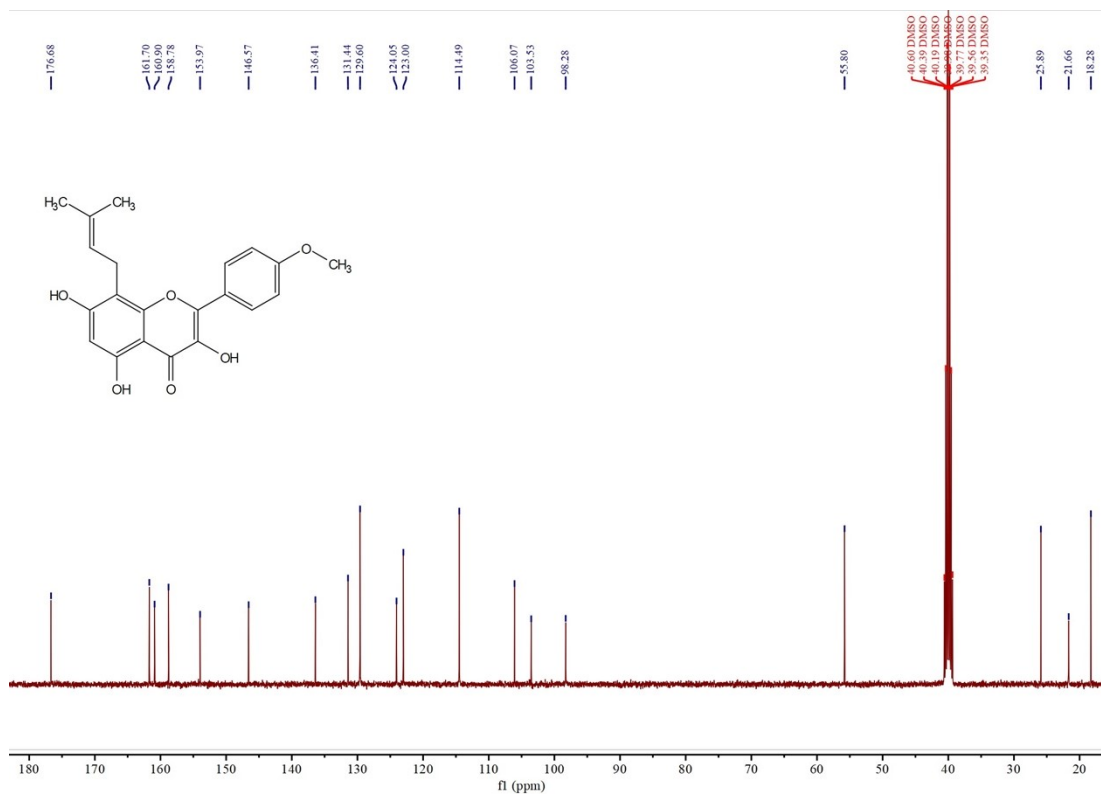


Figure S2. $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$) chart of icaritin.

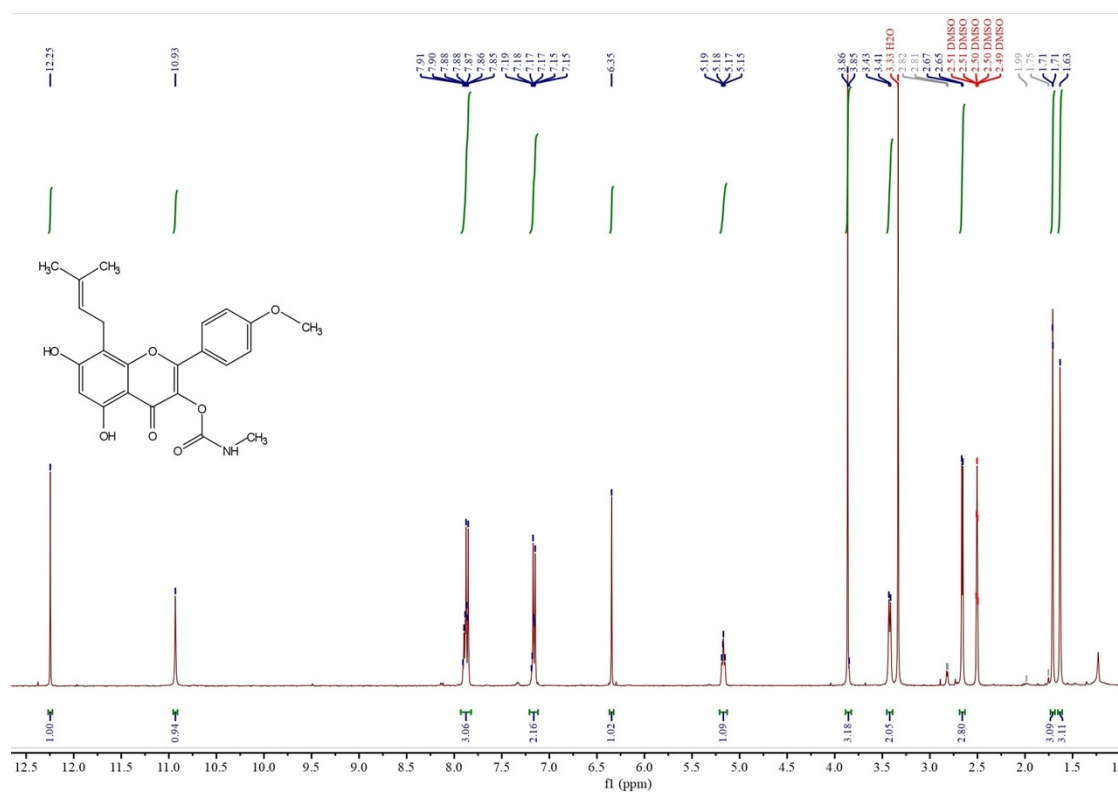


Figure S3. ¹H-NMR (DMSO-*d*₆) chart of 3N-Me.

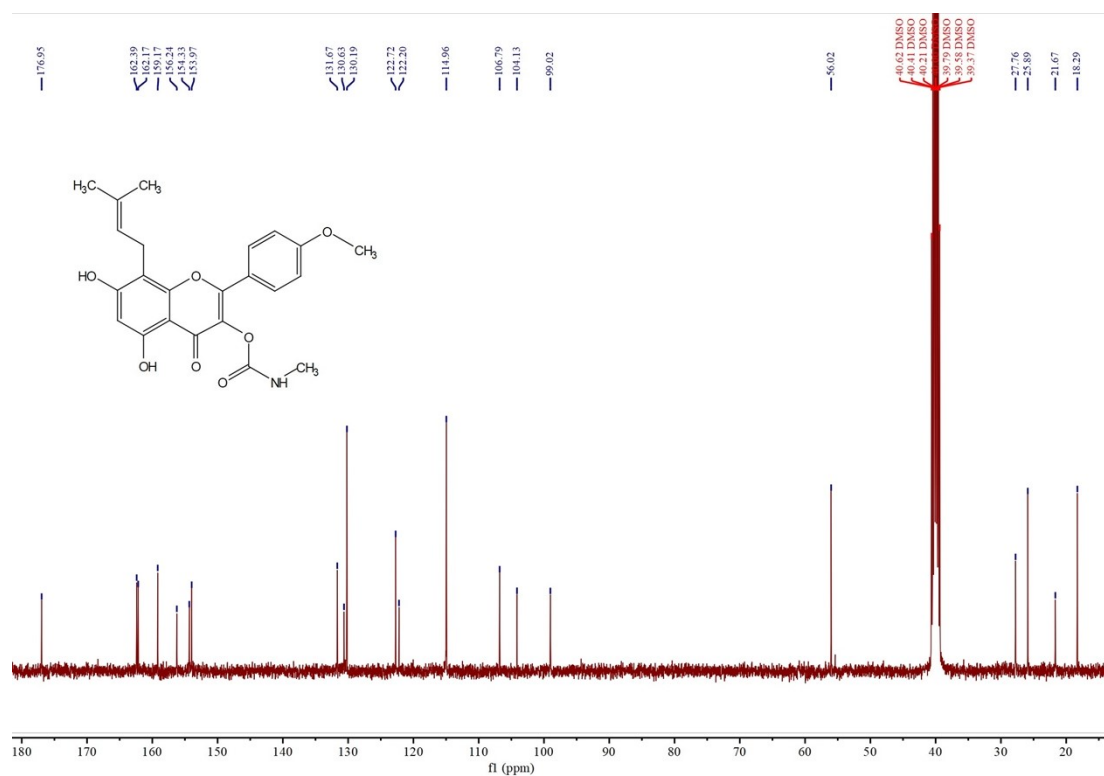


Figure S4. ¹³C-NMR (DMSO-*d*₆) chart of 3N-Me.

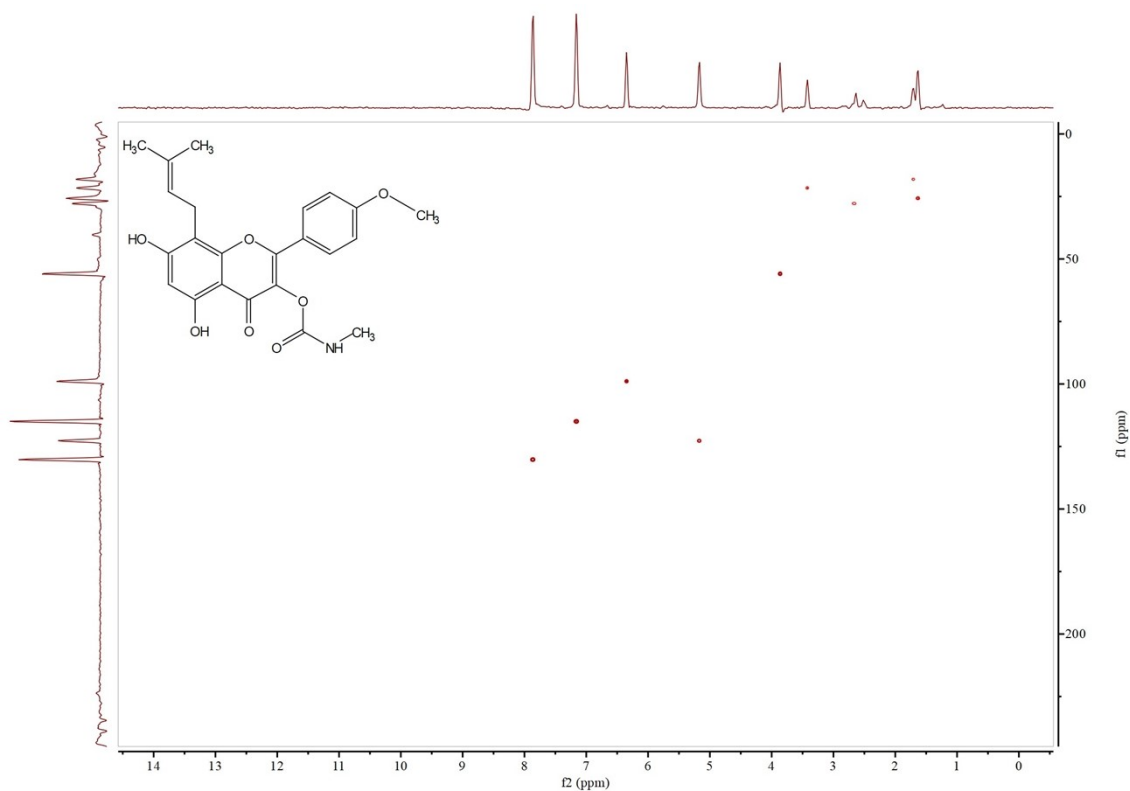


Figure S7. HSQC (DMSO- d_6) chart of 3N-Me.

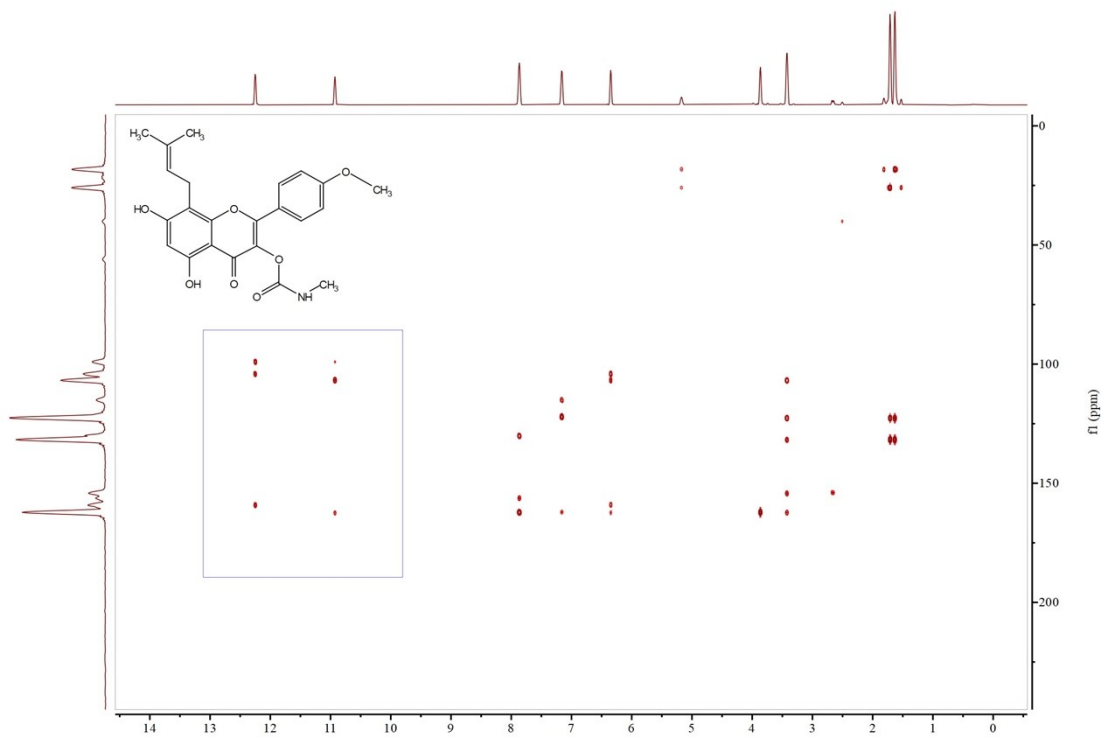


Figure S8. HMBC (DMSO- d_6) chart of 3N-Me.

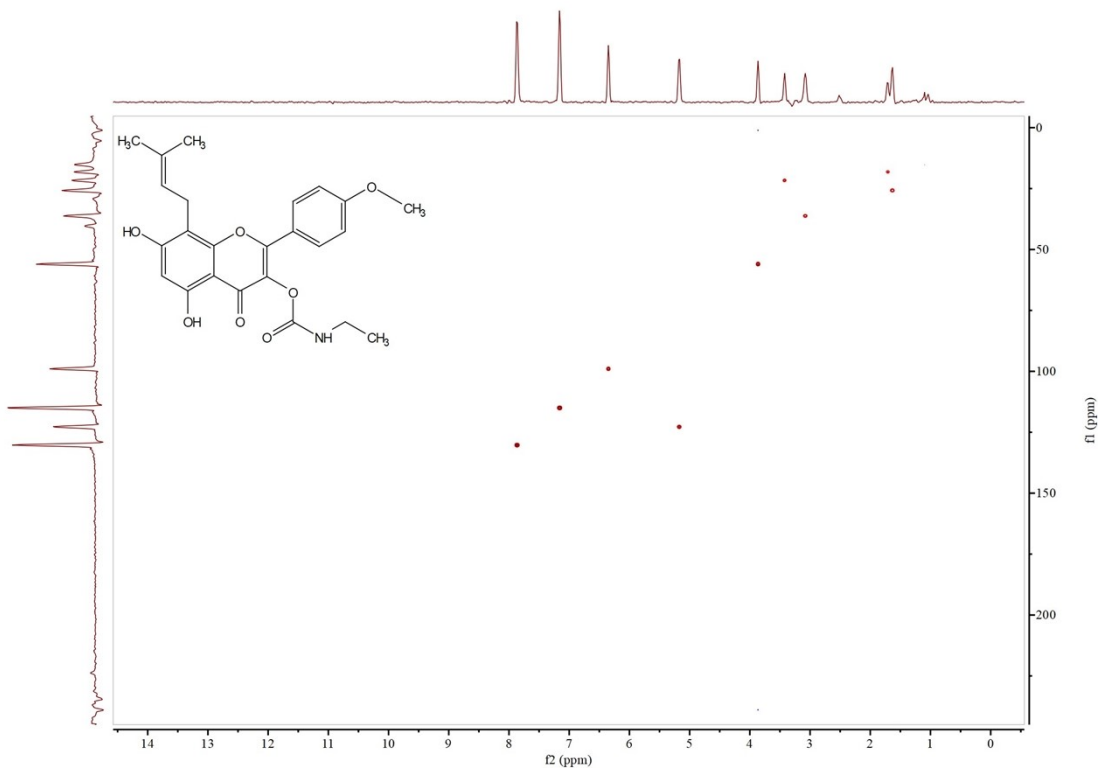


Figure S9. HSQC (DMSO- d_6) chart of 3N-Et.

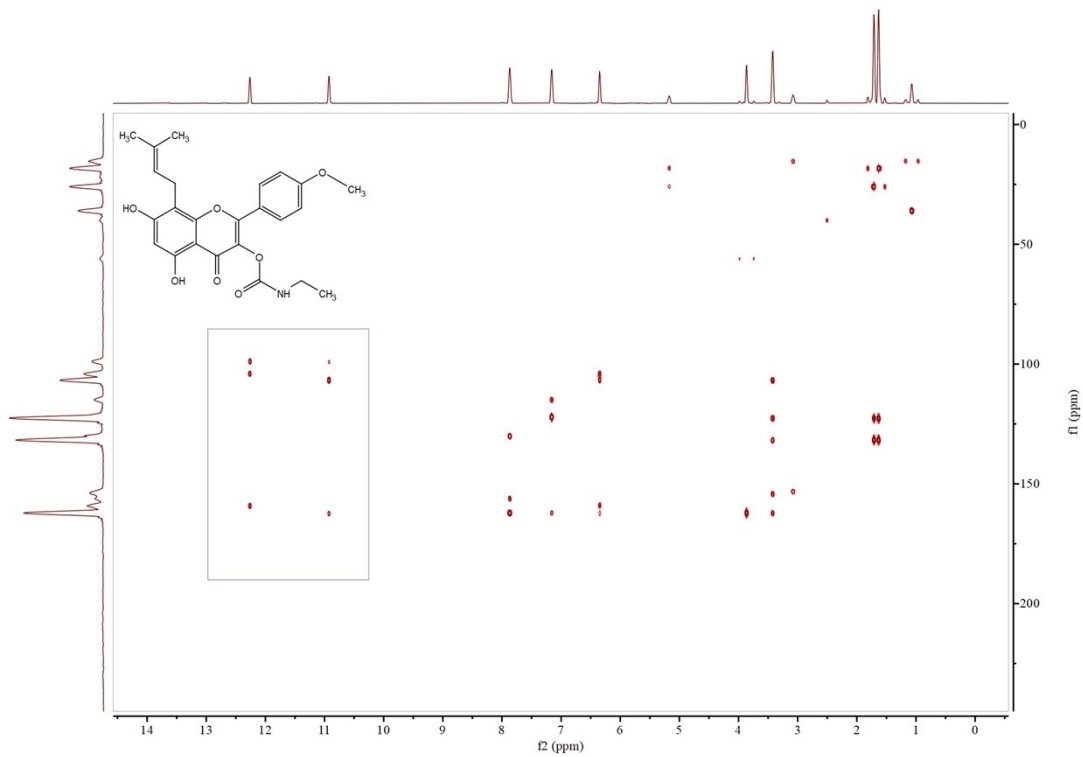


Figure S10. HMBC (DMSO- d_6) chart of 3N-Et.

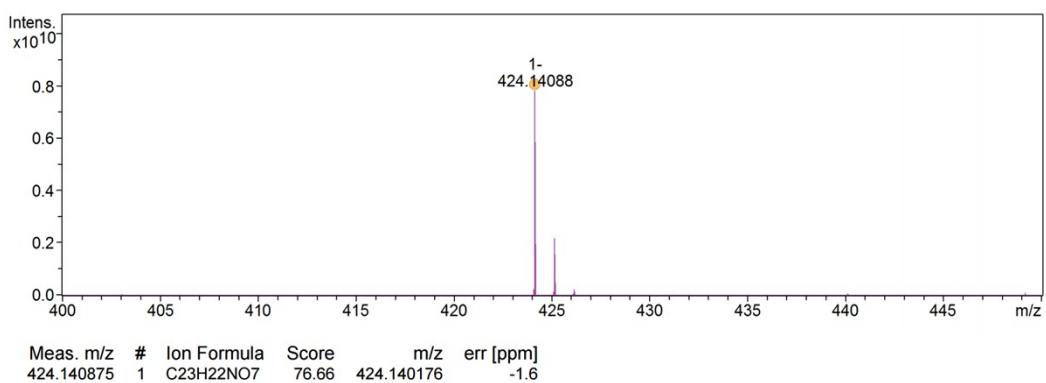


Figure S11. HRMS chart of 3N-Me.

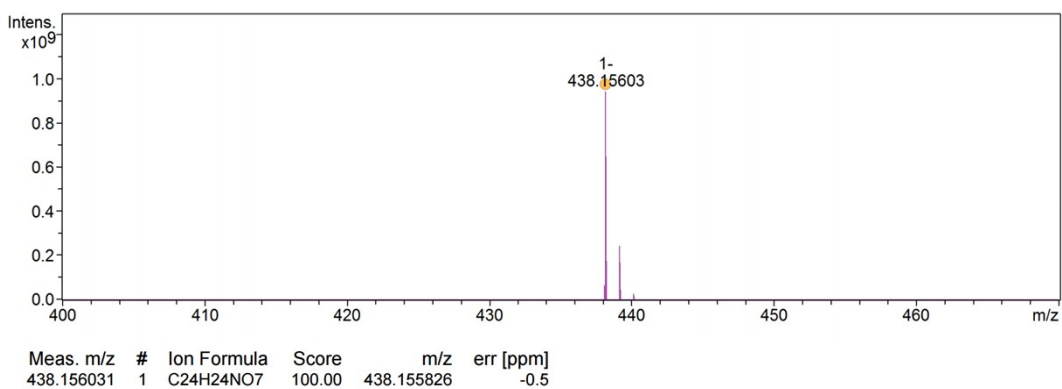


Figure S12. HRMS chart of 3N-Et.

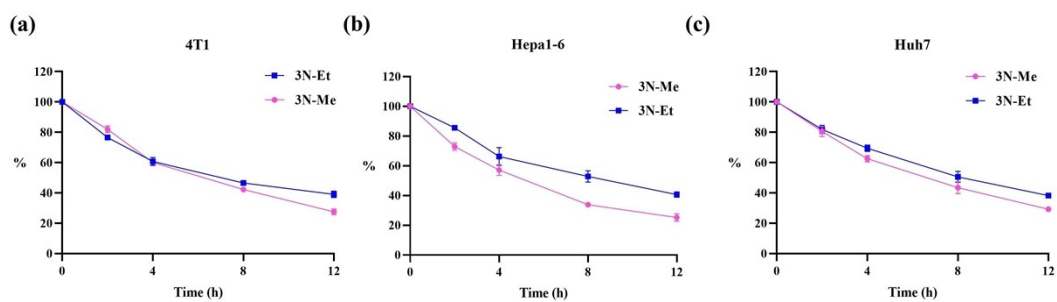


Figure S13. The stability of 3N-Me and 3N-Et in tumor cells (n = 3). (a) 4T1 cells; (b) Hepa1-6 cells; (c) Huh7 cells.

Table S1. The half-life ($t_{1/2}$) of 3N-Me and 3N-Et in different tumor cells

$t_{1/2}$ (h)	4T1	Hepa1-6	Huh7
3N-Me	6.42	5.99	6.61
3N-Et	9.08	9.29	8.19