

Identification of RBPJ-specific inhibitors for blocking Notch signaling in breast cancer using drug repurposing strategy

Mengjie Rui¹, Min Cai¹, Yu Zhou¹, Wen Zhang¹, Lianglai Gao¹, Ke Mi¹, Wei Ji¹, Dan Wang¹, Chumley Feng^{1,*}

¹ Department of Pharmaceutics, School of Pharmacy, Jiangsu University, Zhenjiang 212013, PR China; mjrui@ujs.edu.cn (M. R.); 2211915001@stmail.ujs.edu.cn (M. C.); 2221815020@stmail.ujs.edu.cn (Y. Z.); 2221915025@stmail.ujs.edu.cn (W. Z.); 2222015007@stmail.ujs.edu.cn (L. G.); 2212015010@stmail.ujs.edu.cn (K. M.); jinjian@ujs.edu.cn (W. J.); danwang@ujs.edu.cn (D. W.); feng@ujs.edu.cn (C. F.)

*Correspondence: feng@ujs.edu.cn;

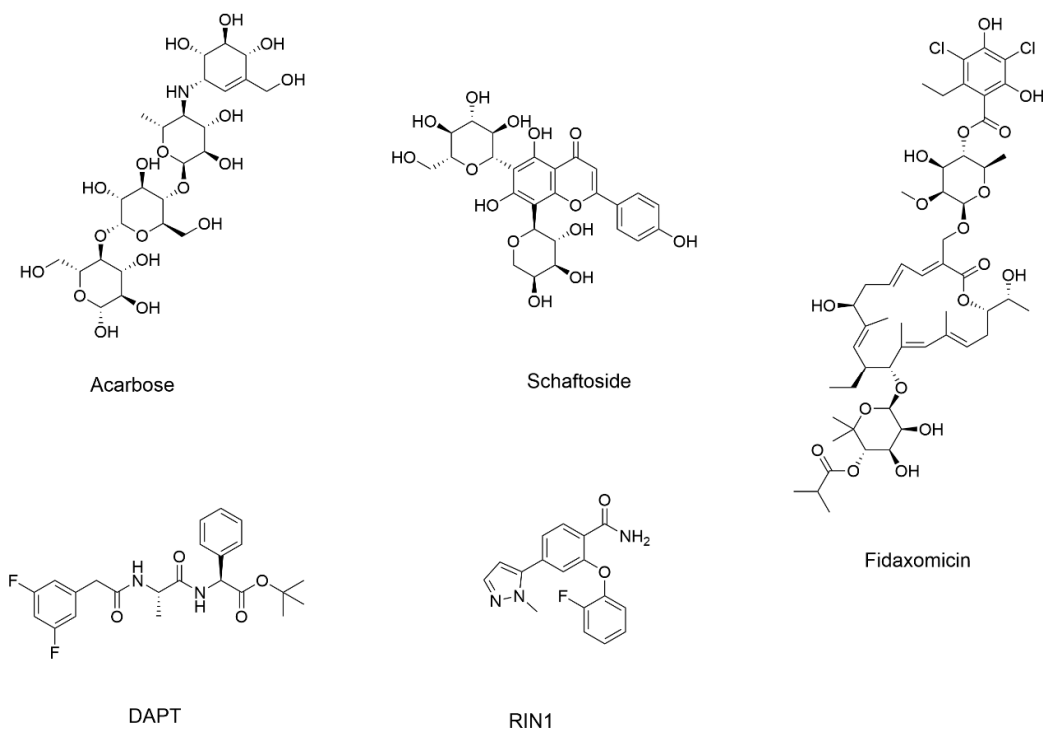


Figure S1. The chemical structures of compounds used in this study.

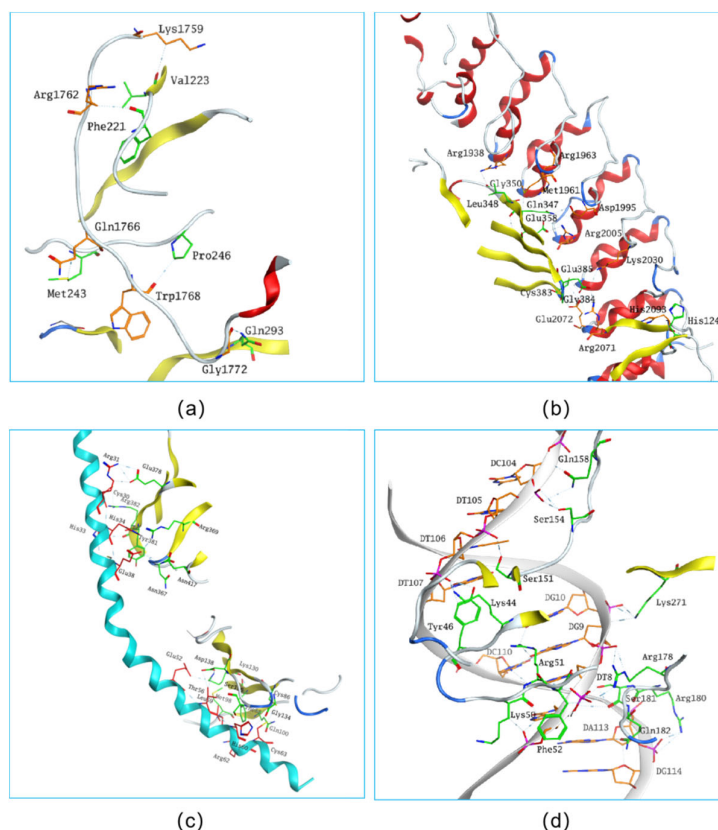


Figure S2. Schematic diagram of the interaction between Notch, MAML, DNA and RBPJ. (a) shows the schematic diagram of the interaction between RAM domain and RBPJ in Notch receptor. (b) shows the schematic diagram of the interaction between the ANK domain and RBPJ in the Notch receptor. (c) shows the schematic diagram of the interaction between DNA and RBPJ. (d) represents the schematic diagram of the interaction between MAML and RBPJ.

Table S1 Interactions between human transcription factor RBPJ and NICD

Residues of NICD	Residues of RBPJ	Interactions
Lys1759	Val223	H-bond
Arg1762	Phe221	H-bond
Gln1766	Met243	H-bond
Trp1768	Pro246	H-bond
Gly1772	Gln293	H-bond
Arg1938	Gly350	H-bond

Met1961、Met1993、Asp1995	Gln347	H-bond
Arg1963	Leu348	H-bond
Arg2005	Glu358	H-bond
Lys2030	Glu385	H-bond
Glu2072	Cys383、Gly384	H-bond
His2093、Met2094	His124	H-bond

Table S2 Interactions between human transcription factor RBPJ and coactivator
MAML

Residues of MAML	Residues of RBPJ	Interactions
Cys30	Arg382	H-bond
Arg31	Arg378	H-bond
His33	Arg382	H-bond
His34	Tyr381	H-bond
Glu38	Asn367、Arg369、Asn417	H-bond
Glu52	Lys130	H-bond
Thr56	Lys130、Asp138	H-bond
Leu59	Phe88	p- π conjugation
His60	Gly134、Ser136	H-bond、p- π conjugation
Arg62	Met98	H-bond
Cys63	Cys86	H-bond

Table S3 Primer sequence

Primer	Sequences (5' to 3')
GAPDH-F	GGTTGTCTCCTGCGACTTCA
GAPDH-R	TGGTCCAGGGTTTCTTACTCC
Notch1-F	AGACCAACATCAATGAGTGCCACAG
Notch1-R	GCATAAGCAGAGGTAGGAGTTGTCAC
Hes1-F	GAGGCGAAGGGCAAGAATAAATGAAAG
Hes1-R	AATGTCTGCCTTCTCTAGCTTGGAATG
Hes5-F	GCATGTGGGCACGATTTTGTACTTAG
Hes5-R	ATTAGAAGCCTTCAGAACAGCCTGTG

Hey1-F	GAAAGGTGTCTGTGCCCTGAATCC
Hey1-R	CATAACTGTCTTGCTTGCTGCCAAC
