

Table S1 The information for laryngeal squamous cell carcinoma and TFA shared targets.

Gene	Uniprot	Gene Full Name	Protein Class	Degree	FC
EGFR	P00533	epidermal growth factor receptor	tyrosine-protein kinase	9	2.49
ERBB2	P04626	receptor tyrosine-protein kinase erbB-2	tyrosine-protein kinase	7	-2.08
ERBB4	Q15303	receptor tyrosine-protein kinase erbB-4	tyrosine-protein kinase	3	-13.5
MMP1	P03956	matrix metallopeptidase 1	hydrolase; metalloprotease	3	49.49
MMP3	P08254	matrix metallopeptidase 3	hydrolase; metalloprotease	2	13.34
NRAS	P01111	neuroblastoma RAS viral oncogene homolog	enzyme modulator	3	2.50
NOX4	Q9NPH5	NADPH oxidase 4	oxidoreductase	1	2.34
TOP2A	P11388	topoisomerase (DNA) II alpha	DNA-binding; isomerase; topoisomerase	2	3.70
DRD1	P21728	dopamine D1 receptor	G-protein coupled receptor; transducer	2	-2.53
MAOB	P27338	monoamine oxidase B	oxidoreductase	2	-2.70
ACHE	P22303	Acetylcholinesterase	hydrolase	2	-2
CA9	Q16790	carbonic anhydrase 9	lyase	2	12.64

ALDH1A1	P00352	retinal dehydrogenase 1	oxidoreductase	3	-2.50
ALDH1A2	O94788	retinal dehydrogenase 2	oxidoreductase	1	-2.50
ALOX12B	O75342	epidermis-type lipoxygenase 12	oxidoreductase	1	2.11
ALOX15	P16050	arachidonate 15-lipoxygenase	oxidoreductase	1	-2.61
DCT	P40126	dopachrome tautomerase	isomerase	0	-4.54
CYP1B1	Q16678	cytochrome P450 1B1	oxidoreductase	0	-2.46
DAPK1	P53355	death associated protein kinase 1	calmodulin-binding; kinase; serine/threonine- protein kinase	0	2

FC: Fold change, the positive value indicates that the cancer is up-regulated compared with the adjacent cancer, and the negative value indicates that the cancer is down-regulated.

Table S2 Molecular docking results of targets and compounds.

No.	Compounds	Docking number	Targets Symbol (docking score ^a)
1	formononetin	2	MAOB (5.924); ALOX15 (4.817)
2	ononin	13	MAOB (7.772); ALOX15(7.634); TOP2A(7.374); DAPK1 (6.442); EGFR(6.371); ALDH1A2(6.225); ALDH1A1(6.223); MMP3(6.176); ERBB2(5.576); NRAS(5.636); MMP1 (5.562); ACHE (5.513); ERBB4(5.502)
3	calycosin	3	MAOB(5.229); ALOX15(4.547); TOP2A (4.537)
4	calycosin-7-O- β -D-glucoside	13	MAOB(7.774); ALOX15(7.603); TOP2A(6.99); EGFR(6.285);DAPK1(6.269); ALDH1A2(6.201); ALDH1A1(6.143);MMP3(6.144); MMP1(6.048); ACHE(5.566); NRAS(5.386);ERBB2(5.528); ERBB4(5.527)
5	7,2'-dihydroxy-3',4'-dimethoxyisoflavan	4	MAOB(5.414); TOP2A(5.406); ALOX15(5.235); DAPK1(4.675)
6	7,2'-dihydroxy-3',4'-dimethoxyisoflavan eglucoside	13	TOP2A(7.976); MAOB(7.937); ALOX15(7.87); DAPK1(6.775); ALDH1A1(6.412); EGFR(6.4); MMP3(6.344); ALDH1A2(6.276); MMP1(6.189); NRAS(6.155); ACHE (5.733); ERBB2(5.706); ERBB4(5.643)
7	3-hydroxy-9,10-dimethoxypterocarp an	11	MMP3(7.139); ALDH1A2(7.125); ALDH1A1(7.105); DAPK1(6.883); ALOX15(6.806); MMP1(6.741);EGFR(6.467); MAOB(6.061); ERBB2(5.659); ACHE(5.142); ERBB4(4.958)

8	9, 10- dimethoxypterocarp an-3-O- β -D- glucoside	13	TOP2A(8.013); MAOB(7.971); ALOX15(7.92); DAPK1(7.147); NRAS(6.674); ERBB2(6.649); ALDH1A1(6.435); ALDH1A2(6.293); MMP3(6.28); MMP1(6.136);ACHE(5.675); EGFR(5.666); ERBB4(5.657)
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a: The results were screened out with docking score >4.52.