

Table S1 The specific information about the relationship between the compounds and corresponding mode of action

Compounds	Compounds_count	MoA	MoA_sum_count
estriol	1	Estrogen receptor agonist	82
nepafenac	1	Cyclooxygenase inhibitor	193
JLK-6	2	Gamma secretase inhibitor	12
JLK-6	2	Beta amyloid inhibitor	5
amrinone	1	Phosphodiesterase inhibitor	127
BRD-K04923131	2	GSK inhibitor	64
BRD-K04923131	2	Lipoxygenase inhibitor	46
laropiprant	1	Prostanoid receptor antagonist	44
telcagepant	1	Calcitonin antagonist	7
UB-165	1	Acetylcholine receptor agonist	52
SB-258585	1	Serotonin receptor antagonist	279
sulfinpyrazone	1	Uricosuric	7
icariin	1	Phosphodiesterase inhibitor	127
tazarotene	1	Retinoid receptor agonist	57
SN-38	1	Topoisomerase inhibitor	61
etomoxir	1	Carnitine palmitoyltransferase inhibitor	8
SB-206553	1	Serotonin receptor antagonist	279
CP-466722	1	ATM kinase inhibitor	13
epirizole	1	Cyclooxygenase inhibitor	193
safinamide	3	Dopamine receptor antagonist	244
safinamide	3	Glutamate inhibitor	13
safinamide	3	Monoamine oxidase inhibitor	41
glycitein	1	TNF inhibitor	23
anpirtoline	1	Serotonin receptor agonist	23