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Supplemental information

Global profiling of AMG510 modified proteins identified tumor suppressor KEAP1 as an off-target

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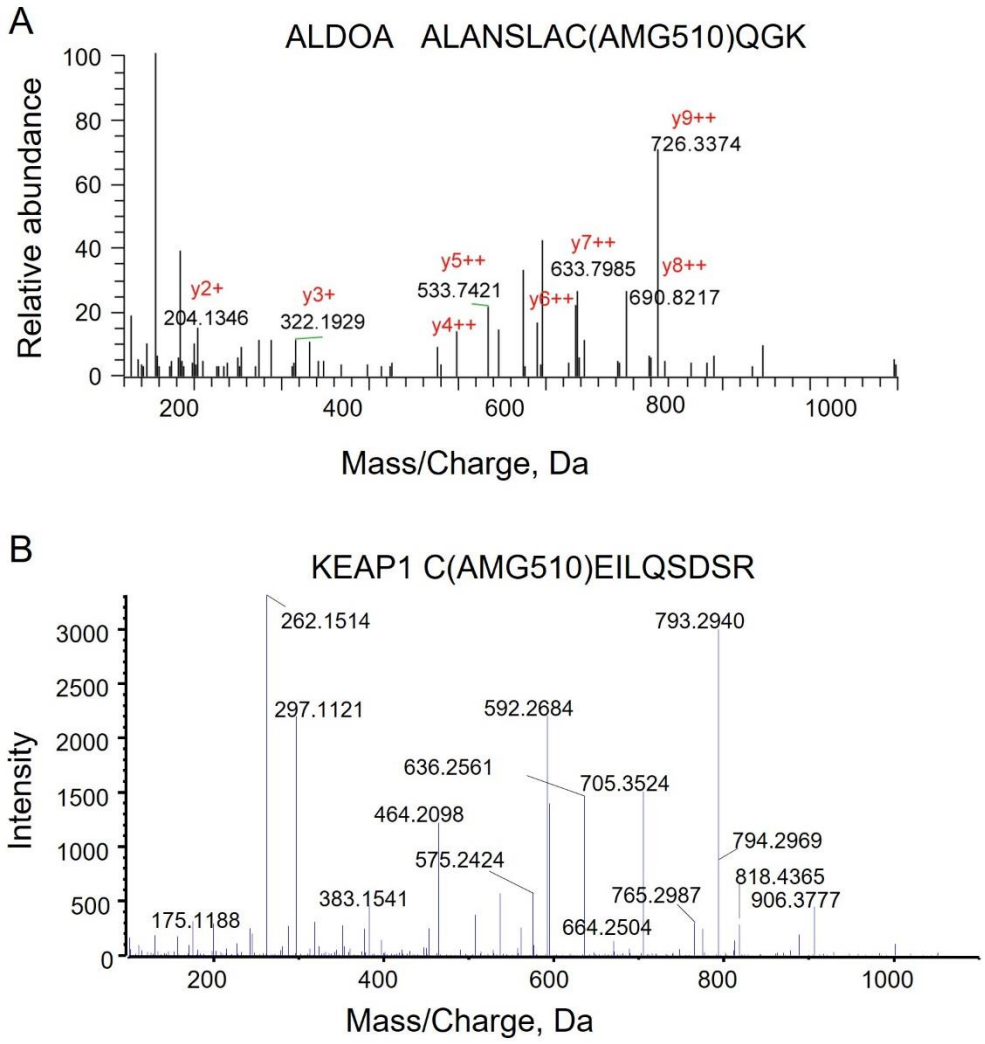
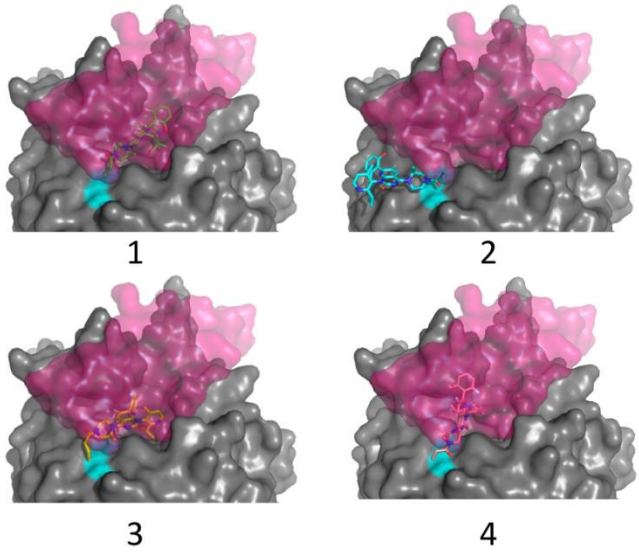


Figure S1 (Related to Figure 6 and 7). AMG510 modified glycolytic enzyme ALDOA. (A) MS/MS spectrum of the peptide in ALDOA containing the AMG510-adducted Cys339. An increment of 560.23 Da, the molecular mass of AMG510, in the peptide fragment containing Cys339 was observed. (B) To analyse KEAP1 modification directly, we synthetized KEAP1 peptide (CEILQSDSR) and incubated with AMG510. The MS/MS of KEAP1 revealed that an increment of 560.23 Da, in the peptide fragment containing Cys288.

A



B

mode	affinity (kcal/mol)	best rmsd	clust. rmsd	ref. rmsd
1	-3.7	0.00	0.0	-1.0
2	-3.7	0.00	15.8	-1.0
3	-3.5	0.00	12.8	-1.0
4	-3.5	0.00	11.8	-1.0

Figure S2 (Related to Figure 6). RAE1-AMG510 docking analysis result. (A) The four highest-scored models of RAE1·AMG510 were simulated by using AutoDockFR (AutoDock for Flexible Receptors). (B) The detailed scores of the above four models.