

**Figure S1** Compound-disease regulatory networks showing the targeted relationship between the Amadori compounds and the intersection genes. (A) Glucose-Amadori compounds; (B) Maltose-Amadori compounds.

	Glucose									GLC-TRP								maltose								MAL-TRP							
Target ID	Vina	Cavity	Center			Size		Vina	Cavity		Center		Size			Vina	Cavity	Center			Size			Vina	Cavity		Center		Size				
	score	size	х	У	Z	х	У	z	score	size	х	У	Z	х	У	z	score	size	х	У	z	х	У	Z	score	size	х	У	Z	х	У	Z	
VEGFA (PDB:4KZN)	-4.5	43	-14	1	3	16	16	16	-5.9	25	7	-2	16	24	24	24	-4.9	43	-14	1	3	20	20	20	-6.1	25	7	-2	16	27	27	27	
	-4.1	25	7	-2	16	16	16	16	-5.8	43	-14	1	3	24	24	24	-4.7	25	7	-2	16	20	20	20	-6	43	-14	1	3	27	27	27	
	-3.9	39	28	-2	14	16	16	16	-5.8	22	22	5	10	24	24	24	-4.3	46	18	-1	16	20	20	20	-5.9	46	18	-1	16	27	27	27	
	-3.9	22	22	5	10	16	16	16	-5.7	46	18	-1	16	24	24	24	-4	39	28	-2	14	20	20	20	-5.4	39	28	-2	14	27	27	27	
	-3.4	46	18	-1	16	16	16	16	-4.9	39	28	-2	14	24	24	24	-4	22	22	5	10	20	20	20	-5.4	22	22	5	10	27	27	27	
CASP3 (PDB:1QX3)	-4.5	266	-3	31	14	16	16	16	-7.2	266	-3	31	14	24	24	24	-5.8	266	-3	31	14	20	20	20	-7.7	266	-3	31	14	27	27	27	
	-4.5	86	21	45	9	16	16	16	-6.6	86	21	45	9	24	24	24	-5.4	696	13	35	-13	20	20	20	-7.2	696	13	35	-13	27	27	27	
	-4.2	696	13	35	-13	16	16	16	-6.5	696	13	35	-13	24	24	24	-5	389	7	47	10	20	20	20	-6.6	86	21	45	9	27	27	27	
	-4.2	139	16	52	-6	16	16	16	-5.8	139	16	52	-6	24	24	24	-5	86	21	45	9	20	20	20	-6.4	139	16	52	-6	27	27	27	
	-3.7	389	7	47	10	16	16	16	-5.3	389	7	47	10	24	24	24	-4.7	139	16	52	-6	20	20	20	-5.7	389	7	47	10	27	27	27	
SRC (PDB:2SRC)	-5.6	877	18	27	58	16	16	16	-8.2	405	11	19	59	24	24	24	-7	405	11	19	59	20	20	20	-9.5	877	18	27	58	27	27	27	
	-5.5	676	27	45	80	16	28	24	-8.1	877	18	27	58	24	24	24	-6.7	877	18	27	58	20	20	20	-9.2	405	11	19	59	27	27	27	
	-5.4	709	34	45	63	16	16	16	-8	709	34	45	63	24	24	24	-6.6	676	27	45	80	20	28	20	-8.4	709	34	45	63	27	27	27	
	-5.3	405	11	19	59	16	16	16	-8	676	27	45	80	24	24	24	-6.4	709	34	45	63	20	20	20	-8.1	676	27	45	80	27	27	27	
	-5.2	413	19	42	56	16	16	22	-7.2	413	19	42	56	24	24	24	-6.4	413	19	42	56	20	20	20	-8.1	413	19	42	56	27	27	27	

Table S1 First 5 vina scores and cavity information of the docking simulation pose for Amadori compounds/carbohydrates and targeted proteins



**Figure S2** Schematic diagram of molecular docking. (A) Vascular endothelial growth factor A-Glucose; (B) Vascular endothelial growth factor A-Glucose-Tryptophan; (C) Vascular endothelial growth factor A-Maltose; (D) Vascular endothelial growth factor A-Maltose-Tryptophan; (E) Caspase-3-Glucose; (F) Caspase-3-Glucose-Tryptophan; (G) Caspase-3-Maltose; (H) Caspase-3-Maltose-Tryptophan; (I) Proto-oncogene tyrosine-protein kinase Src-Glucose; (L) Proto-oncogene tyrosine-protein kinase Src-Maltose; (L) Proto-oncogene tyrosine-protein kinase Src-Maltose-Tryptophan.