

Table S7 Binding energy of AGEs, quercetin, and caffeic acid to RAGE

	Binding energy (kcal/mol)									
	1	2	3	4	5	6	7	8	9	10
Pyrrole-RAGE	-3.81	-2.92	-2.65	-2.22	-2.04	-1.69	-1.60	-1.16	-1.12	-1.10
CEL-RAGE	-1.73	-1.35	-0.87	-0.43	-0.34	+0.09	+0.40	+0.82	+0.83	+1.01
CML-RAGE	-1.80	-0.76	-0.75	-0.68	-0.51	-0.48	-0.09	-0.06	+0.62	+1.35
Quercetin-RAGE	-4.94	-4.78	-4.68	-4.55	-4.15	-4.10	-4.01	-3.88	-3.73	-3.51
Caffeic acid-RAGE	-5.28	-5.27	-5.21	-4.84	-4.78	-5.17	-5.01	-4.66	-4.62	-4.32
CEL-caffeic acid-quercetin-RAGE	-9.98	-9.96	-9.86	-9.75	-9.46	-9.43	-9.29	-9.19	-9.19	
CML-caffeic acid-quercetin-RAGE	-8.76	-8.53	-8.46	-8.34	-8.33	-8.32	-8.03	-7.95	-7.89	
Pyrrole-caffeic acid-quercetin-RAGE	-10.00	-9.99	-9.96	-9.83	-9.75	-9.69	-9.66	-9.62	-9.60	