Tab. S7 Binding affinities of compounds to proteins computed with the MM-GBSA method (ΔG: kcal/mol).					
Systems	ΔE_{ele} [a]	ΔE_{vdw} [b]	ΔG_{pol} [c]	ΔG_{nonpol} [d]	$\Delta G_{MM/GBSA}$ [e]
STAT3-quercetagetin	-44.26±16.97	-15.75±6.48	51.03±12.63	-3.15±0.50	-12.14±3.24
TNF-α-4-(3-Phenylacryloyloxymethyl)-6,7-dimethoxycoumarin	-10.34±2.79	-53.84±2.40	29.04±2.29	-6.92±0.24	-42.06±3.83

[a] ΔE_{ele} stood for the electrostatic energy contribution

[b] ΔE_{vdw} represented van der Waals interactions contribution

[c] ΔG_{pol} was the polar solvent interaction energy calculated by GB model

[d] ΔG_{nonpol} was nonpolar solvation free energy, which was evaluated using LCPO method

[e] $\Delta G_{MM/GBSA}$ represented binding free energy, $\Delta G_{MM/GBSA} = \Delta E_{vdw} + \Delta E_{ele} + \Delta G_{pol} + \Delta G_{nonpol}$