

Table S8 Standard system formation enthalpy difference before and after ligand binding

| Ligand                | Quercetin | Quercetin | Quercetin | Quercetin | Quercetin | Quercetin | Caffeic acid |
|-----------------------|-----------|-----------|-----------|-----------|-----------|-----------|--------------|
| Target protein        | CCL2      | CXCL8     | F3        | ICAM1     | IL6       | SELE      | TNF          |
| Receptor              | CCR2      | CXCR1     | TFR1      | LFA-1     | IL6R      | PSGL-1    | TNFR1        |
| $\Delta H$ (kcal/mol) | 294.75    | 203.57    | 180.60    | 233.75    | 275.95    | 303.42    | 290.26       |