***Table S1.*** Binding constants (*K*a, M-1), thermodynamic parameter (Δ*H*, kcal mol-1) and *C* values for **WP6** and guests. Conditions: 1× PBS buffer, 298 K.

|  |  |  |
| --- | --- | --- |
| Guest | *Ka* with **WP6** (M-1); Δ*H* and *C or app. C* | *Duplicate Ka* with **WP6** (M-1); Δ*H* and *C or app. C* |
| **G1***a* | (5.29 ± 0.07) × 104; −8.08 ± 0.02;*26* | (5.15 ± 0.16) × 104; −7.87 ± 0.03;*27.1* |
| **G2***b* | (4.59 ± 0.35) × 107; −6.10 ± 0.02;*172* | (4.48 ± 0.21) × 107; −6.15 ± 0.02;*167* |
| (±)-**G3***a* | (6.45 ± 0.18) × 105; −4.75 ± 0.02;*64.5* | (6.25 ± 0.30) × 105; −4.68 ± 0.02;*62.7* |
| **G4***e* | (5.08 ± 0.11) × 104; −4.15 ± 0.02;*25.4* | (4.97 ± 0.16) × 104; −3.98 ± 0.02;*26.3* |
| **G5***f* | (9.01 ± 0.23) × 103; −3.95 ± 0.03;*9* | (9.31 ± 0.22) × 103; −4.15 ± 0.03;*4.2* |
| **G6***c* | (7.09 ± 0.44) × 105; −6.90 ± 0.07;*35.5* | (7.26 ± 0.44) × 105; −7.10 ± 0.04;*36.1* |
| **G7***d* | (1.31 ± 0.05) × 105; −3.18 ± 0.02;*26.2* | (1.29 ± 0.05) × 105; −3.17 ± 0.02;*25.7* |
| **G8***e* | (2.35 ± 0.04) × 104; −9.55 ± 0.05;*11.7* | (2.30 ± 0.06) × 104; −9.51 ± 0.05;*11.5* |
| **G9***f* | (3.75 ± 0.31) × 104; −5.31 ± 0.08;*37.4* | (3.68 ± 0.37) × 104; −5.21 ± 0.08;*36.8* |
| **G10***b* | (1.61 ± 0.08) × 107; −6.23 ± 0.02;*59.1* | (1.60 ± 0.12) × 107; −6.11 ± 0.02;*63* |
| **G11***f* | (3.37 ± 0.05) × 104; −5.61 ± 0.02;*33.7* | (3.31 ± 0.05) × 104; −5.45 ± 0.03;*33.1* |
| (±)-**G12***g* | (9.43 ± 0.31) × 107; −7.45 ± 0.02;*142* | (8.40 ± 0.51) × 107; −7.41 ± 0.02;*309* |
| **G13***c* | (1.63 ± 0.11) × 106; −4.98 ± 0.04;*81.3* | (1.61 ± 0.11) × 106; −4.96 ± 0.03;*82* |

*a* Measured directly by ITC during the titration of **WP6** (0.1 mM) in the cell with guest (1 mM) in the syringe. *b* Measured by the ITC competition titration by mixing **G7** (0.2 mM) and **WP6** (0.1 mM) in the cell with guest (1 mM) in the syringe. *c* Measured directly by the ITC during the titration of **WP6** (0.05 mM) in the cell with guest (0.5 mM) in the syringe. *d* Measured directly by the ITC during the titration of **WP6** (0.2 mM) in the cell with guest (2 mM) in the syringe. *e* Measured directly by the ITC during the titration of **WP6** (0.5 mM) in the cell with guest (5 mM) in the syringe. *f* Measured directly by the ITC during the titration of **WP6** (1 mM) in the cell with guest (10 mM) in the syringe. *g* Measured by the ITC competition titration by mixing **G7** (0.5 mM) and **WP6** (0.1 mM) in the cell with guest (1 mM) in the syringe.