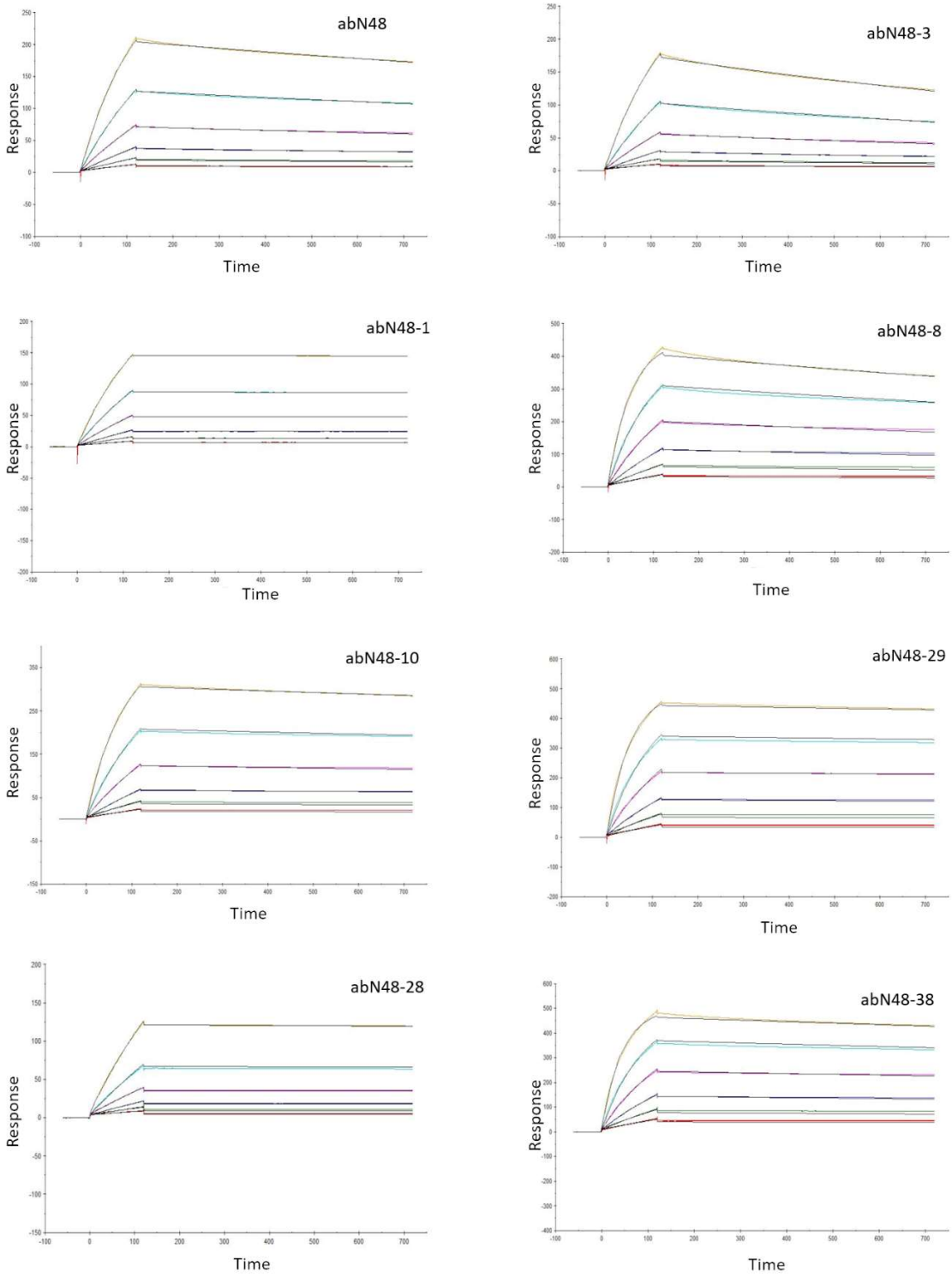


**Figure S1**: Sensorgrams of abN48 and the affinity maturated antibodies binding to and disassociation from human CXCR2 pepN48 peptide, measured by Biacore T200. Lines of different colors correspond to raw data obtained for different antibody concentrations (red curve: 0.2 nM, green curve: 0.5 nM, blue curve: 1 nM, magenta curve: 2 nM, cyan curve: 5 nM, yellow curve: 10

nM ), while the black lines correspond to the best global fit). Kinetics and affinity shown in Figure 1 and Table 2 were calculated from these results.

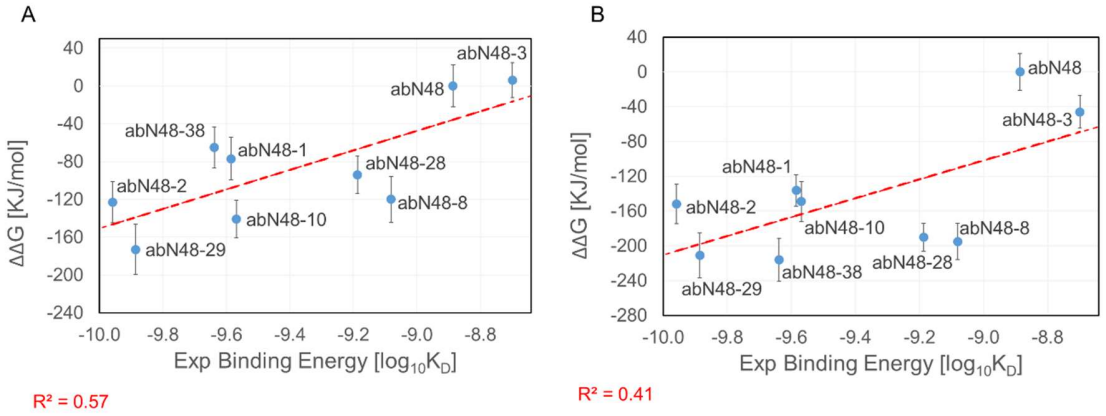


**Figure S2:** Comparison between experimental binding affinities (Figure S1) and binding free energies computed from configurations sampled according to two different schemes: (A) 10 replicas of 2 ns MD simulations are performed and configurations are extracted every 10 ps from the second half of each replica; (B) a single 25 ns MD simulation is performed and configurations are extracted every 10 ps from the last 20 ns of the trajectory. Both sampling schemes show a fair correlation with experimental data, with scheme A being slightly better.

| | CDR-3 Sequence | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | **100** | **101** | **102** | **103** | **104** | **105** | **106** | **107** | **108** | **109** | **110** |
| abN48 | GLY | TYR | CYS | SER | SER | THR | SER | CYS | TYR | ASP | TYR |
| abN48-1 | GLY | PHE | CYS | THR | ARG | THR | ILE | CYS | PHE | VAL | TYR |
| abN48-2 | GLY | TYR | CYS | SER | ARG | THR | ARG | CYS | TYR | ASP | TYR |
| abN48-3 | GLY | TYR | CYS | SER | PHE | ALA | ILE | CYS | PHE | ASP | SER |
| abN48-8 | GLY | TYR | CYS | ASN | ARG | THR | ARG | CYS | TYR | ASP | HIS |
| abN48-10 | GLY | TYR | CYS | SER | ARG | PHE | ASN | CYS | LYS | ASP | TYR |
| abN48-28 | GLY | TYR | CYS | SER | PRO | SER | GLY | CYS | TYR | VAL | TYR |
| abN48-29 | GLY | TYR | CYS | GLY | ARG | ALA | ARG | CYS | THR | SER | PHE |
| abN48-38 | GLY | TYR | CYS | SER | ARG | SER | ARG | CYS | TYR | ASP | TYR |

**Table S1**: Sequences of the antibody used for data in Figure 1