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| **Table S2:** Dynamics of Isoflurane in binding sites |
| **Site** | **Translational diffusion coefficient (Å2/s)** | **Rotational relaxation time (ns)** |
| Water | 100 | 0.1 |
| Extracellular | 2 | 5.3 |
| Linker | 2 | 1 |
| Cavity | 3 | 0.1 |
| Diffusion coefficients and rotational relaxation times of isoflurane computed, at each binding site, by averaging over a trajectory of approximately 500 ns. The water self-diffusion coefficient and the rotational relaxation time for the TIP3P model is reported for comparison.  |