

Table 3. Binding enthalpies (kcal/mol) of the ligands on AR calculated using MD simulations.

Ligand	Ligand binding site (LBS)	AF2 site	BF3 site	In solution (water)
R1881	- 68.3 ± 2.8	- 59.8 ± 3.8	- 55.2 ± 3.6	- 50.6 ± 4.4
DHT	- 67.8 ± 2.9	- 59.6 ± 3.8	- 61.1 ± 4.4	- 53.7 ± 5.1
BPA	- 52.3 ± 3.0	- 52.7 ± 3.6	- 53.3 ± 4.7	- 46.4 ± 3.9
BPAF	- 54.2 ± 3.4	- 50.1 ± 3.1	- 53.4 ± 4.4	- 49.2 ± 3.7
BPS	- 57.7 ± 4.3	- 64.7 ± 5.4	- 65.3 ± 4.4	- 62.2 ± 5.3