

Supplemental; Small compounds modulate and bind MscL similarly

S1Table. List of MM-PBSA free energy components (in kcal/mol) for three top docking poses. ϵ_{lip} is the dielectric constant of the lipids.

System	vdW	EEL	ΔG_{pol}^{PB}			$\Delta G_{nonpolar}^{SAS}$	T Δ s	MM-PBSA		
			$\epsilon_{lip}=1$	$\epsilon_{lip}=2$	$\epsilon_{lip}=4$			$\epsilon_{lip}=1$	$\epsilon_{lip}=2$	$\epsilon_{lip}=4$
Docking Pose 1	-5128.70 \pm 1.97	-46350.91 \pm 5.20	-5467.61 \pm 2.70	-5028.58 \pm 1.10	-4786.99 \pm 3.34	204.30 \pm 0.06	7750.53 \pm 0.57	-64493.46 \pm 7.08	-64054.43 \pm 5.23	-63812.83 \pm 6.16
Docking Pose 3	-5108.47 \pm 4.26	-46619.83 \pm 21.81	-5114.58 \pm 29.76	-4675.69 \pm 28.24	-4426.39 \pm 27.68	206.34 \pm 0.10	7761.97 \pm 0.46	-64398.50 \pm 20.81	-63959.62 \pm 22.02	-63710.32 \pm 22.77
Docking Pose 4	-5112.89 \pm 6.02	-46744.48 \pm 29.90	-4955.35 \pm 7.02	-4536.67 \pm 8.16	-4303.64 \pm 9.45	204.70 \pm 0.03	7756.02 \pm 0.73	-64364.04 \pm 23.37	-63945.35 \pm 22.06	-63712.32 \pm 22.90