Table S1. ΔGDT-HA, ΔRMSD, MolProbity, ΔSphereGrinder values after refinement from sampling in the presence of lipid bilayers with HDGB-based scoring functions using different membrane widths according to predicted hydrophobic lengths.

	1j4n	1py6	1qj8	3odu	3vg9	4hyj	4kr8	4n6h	Ave.
ΔGDT-HA									
HDGBv3-hl	1.21	2.64	10.98	2.07	-2.44	1.48	-2.13	3.13	2.12±1.46
HDGBvdW-hl	1.31	3.42	10.98	1.49	-2.18	1.06	-1.54	3.05	2.20±1.43
ΔRMSD [Å]									
HDGBv3-hl	-0.12	-0.06	-0.45	-0.12	-0.01	-0.06	-0.04	-0.23	-0.14±0.05
HDGBvdW-hl	-0.10	-0.07	-0.45	-0.12	-0.01	-0.06	-0.03	-0.24	-0.13±0.05
MolProbity									
HDGBv3-hl	0.93	0.56	0.65	1.50	0.92	0.78	0.96	0.60	0.86±0.11
HDGBvdW-hl	0.97	0.64	0.65	1.52	0.84	0.78	0.79	0.50	0.84±0.11
HDGBv3-hl	-0.43	0.47	12.15	-1.08	0.18	-1.58	1.35	0.71	1.47±1.56
HDGBvdW-hl	-0.21	0.47	11.8	-1.26	0.54	-1.36	0.9	0.89	1.47±1.51

hl denotes 'hydrophobic length'

Table S2. ΔGDT-HA, ΔRMSD, MolProbity, ΔSphereGrinder values after refinement from sampling in the presence of aqueous solvent with HDGB-based scoring functions using different membrane widths according to predicted hydrophobic lengths.

	1j4n	1py6	1qj8	3odu	3vg9	4hyj	4kr8	4n6h	Ave.
ΔGDT-HA									
HDGBv3-hl	2.51	5.07	8.61	1.24	-0.08	3.81	0.66	-0.17	2.71±1.07
HDGBvdW-hl	2.61	4.63	9.80	1.16	-0.67	3.92	0.88	-0.09	2.78±1.20
ΔRMSD [Å]									
HDGBv3-hl	-0.13	-0.09	-0.33	-0.06	-0.06	-0.11	-0.14	-0.14	-0.13±0.03
HDGBvdW-hl	-0.14	-0.08	-0.34	-0.06	-0.05	-0.12	-0.13	-0.13	-0.13±0.03
MolProbity									
HDGBv3-hl	0.93	1.05	0.97	1.62	0.92	0.87	0.81	0.53	0.96±0.11
HDGBvdW-hl	0.93	0.80	1.05	1.59	0.92	0.92	0.74	0.50	0.93±0.11
SphereGrinder									
HDGBv3-hl	1.1	-0.48	6.59	-1.44	0.36	-1.13	2.41	1.59	1.13±0.91
HDGBvdW-hl	1.75	-1.19	6.59	-1.26	-0.71	-1.36	1.81	1.24	0.86±0.95

hl denotes 'hydrophobic length'