Supporting Information for

Effects of Molecular Weight and Orientation on the Membrane Permeation and Partitioning of Polycyclic Aromatic Hydrocarbons: A Computational Study

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Table S1. The cooperation between calculated parameters from 30-50 ns and the average value

PAHs	P (cm·s^{-1})					τ (ms)					log K_{LW}				
	35-40	40-45	45-50	30-50	average	35-40	40-45	45-50	30-50	average	35-40	40-45	45-50	30-50	average
NAP	12.3	12.8	11.6	11.7	12.1	0.11	0.1	0.14	0.19	0.14	2.57	2.53	2.68	2.81	2.65
PHE	26.2	29.1	24.5	23.1	25.7	2.99	9.67	4.87	2.73	5.06	3.96	4.52	4.27	3.99	4.18
ANT	20.1	16.6	16.4	16.9	17.5	1.16	2.71	5.41	6.51	3.95	3.81	4.08	4.32	4.39	4.15
PYR	20.9	22.1	22.7	19.3	21.2	2.89	7.81	6.84	6.68	6.05	4.24	4.55	4.46	4.42	4.42
CHR	36.8	39.1	38.8	41.2	39.0	359.0	605.9	707	469.9	535	6.49	6.73	6.73	6.58	6.63
BAP	42.5	29.7	31.7	29.2	33.3	3339.3	613.5	475.7	294.8	1180	7.57	6.62	6.49	6.2	6.72
DBA	36.0	35.4	30.4	26.4	32.1	123.2	289.3	269.9	303.4	246	5.81	6.11	6.10	6.05	6.02
COR	35.2	33.1	35.4	32.7	34.1	16805	11878	2254	2858	8449	7.99	7.90	7.21	7.3	7.60

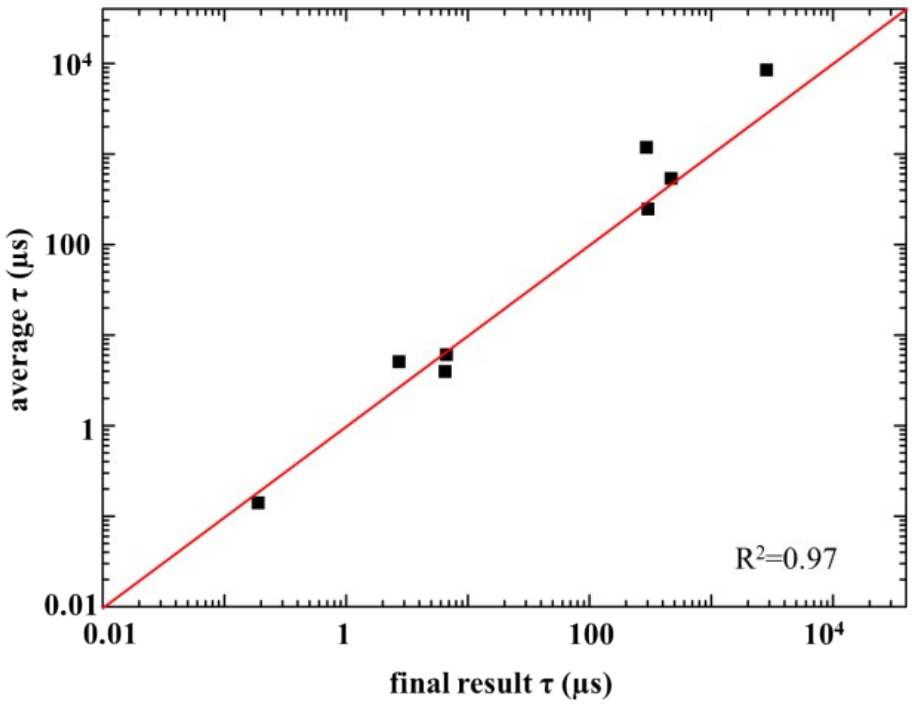

Figure S1. The fitting relationship between our final result of transmembrane time (30-50 ns) and average result (three simulation periods of 35-40 ns, 40-45 ns and 45-20 ns), the red line indicate a 1:1 agreement.

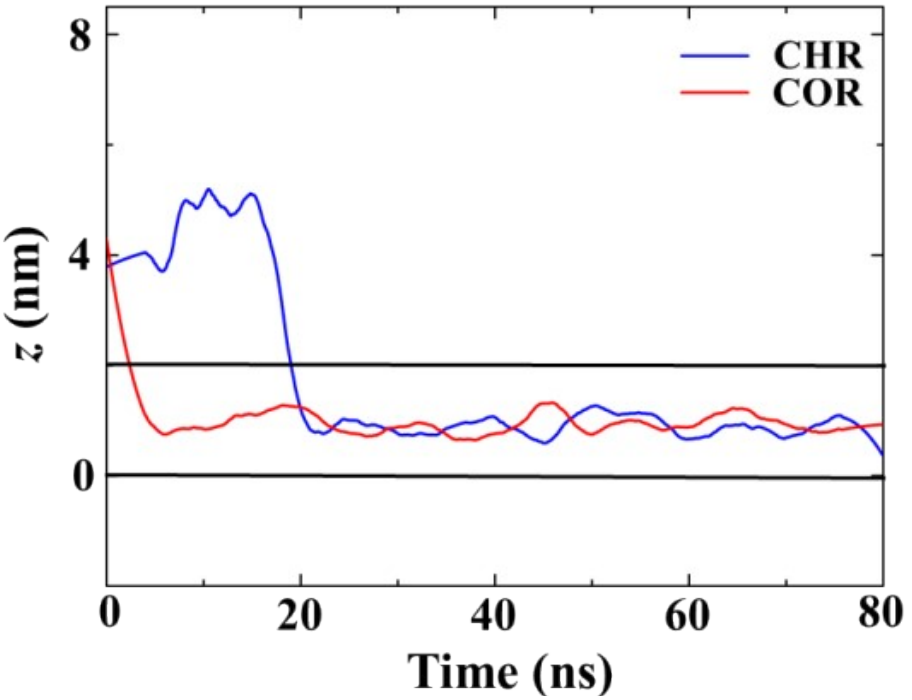

Figure S2. The time evolution of the z position of the center of mass of single CHR (blue line) and COR (red line). The horizontal lines at z = 0 and z = 2 nm represent the center and surface (which was substituted with the average position of the P) of lipid membrane, respectively.

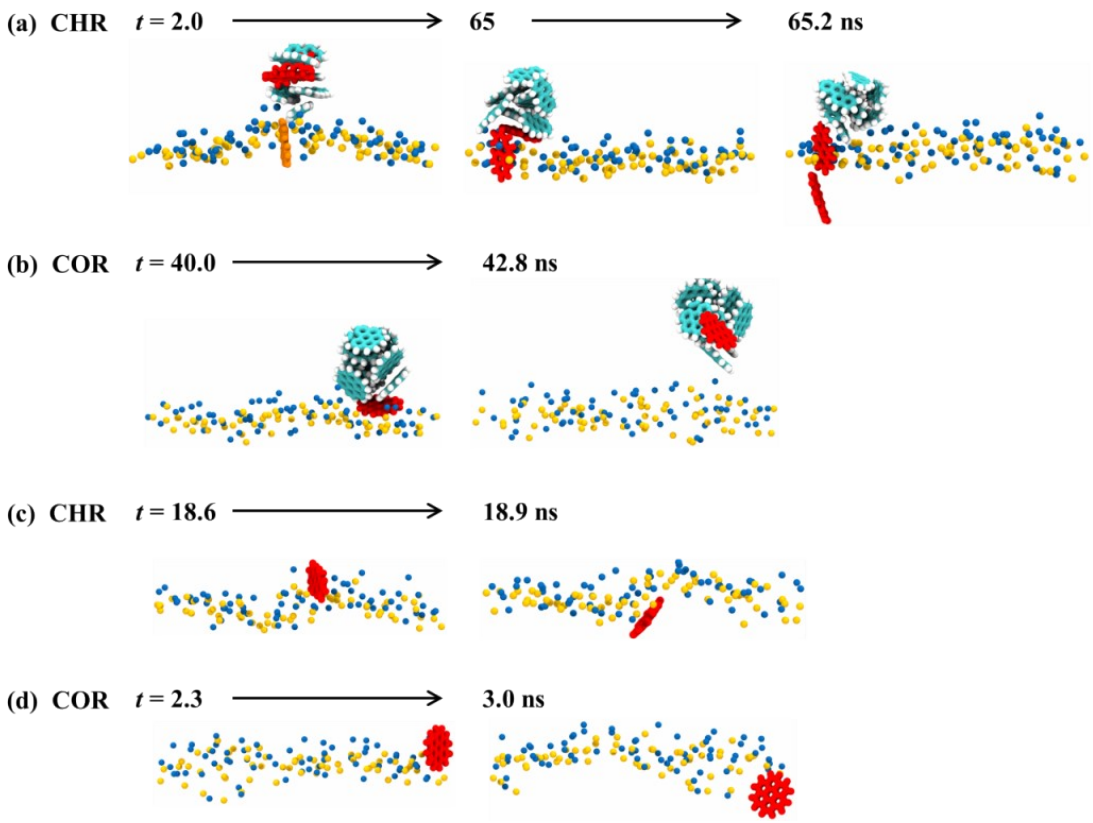

Figure S3. The typical snapshots of the absorption process of (a) CHR, (b) COR. (c) single CHR, (d) single COR.

Table S2. Summary of all simulations performed

	solute	No. of solute	Duration (ns)
Constrained MD	NAP	1	50×32
	PHE	1	50×32
	ANT	1	50×32
	PYR	1	50×32
	CHR	1	50×32
	BAP	1	50×32
	DBA	1	50×32
	COR	1	50×32
Unconstrained MD	NAP	10	80

PYR	10	80
CHR	10	80
COR	10	80
CHR	1	80
COR	1	80