Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

A Relationship between membrane permeation and partition of nitroaromatic explosives and their functional groups. A Computational Study

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Table S1. The free-energy difference and preferred position (z_{min}) of selected nitroaromatic compounds (ΔG_D, ΔG_B, ΔG_{max}, $\Delta G_{max-min}$, $kJ \cdot mol^{-1}$; z_{min}, nm).

Serial number	Compound	ΔG_D	ΔG_B	ΔG_{max}	$\Delta G_{max-min}$	z_{min}
1	1-NB	-10.8	4.6	2.1	12.9	1.05
2	1,2-DNB	-13.2	15.8	2.5	15.8	1.27
3	1,3-DNB	-10.7	13.5	2.8	12.9	1.19
4	1,3,5-TNB	-11.3	25.1	13.7	25	1.35
5	4-NT	-18.3	3.6	1.1	20.6	1.07
6	2,4-DNT	-13.5	15.2	0.6	15.8	1.22
7	2,6-DNT	-14.3	12.3	1.3	15.5	1.19
8	TATB	-12.1	43.3	31.2	43.2	1.57
9	DATB	-10.2	29.2	19	29.2	1.33
10	DNAN	-9.3	20.9	11.6	20.9	1.39
11	2,4-DNP	-11.2	23.9	12.7	23.8	1.25
12	PA	-15.0	45.0	30	45	1.43

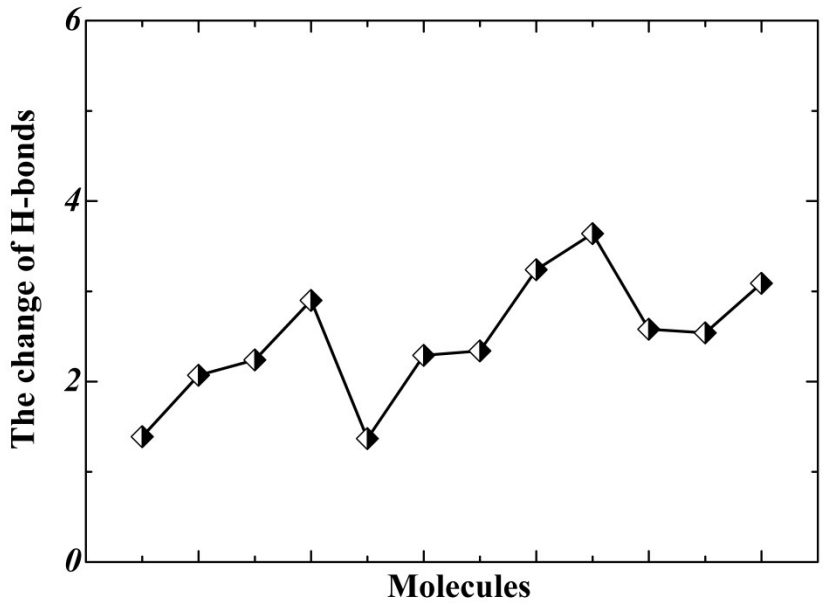

Figure S1. Changes in the number of total H-bonds of all compounds (with water and lipids) from the aqueous phase to the preferred position.

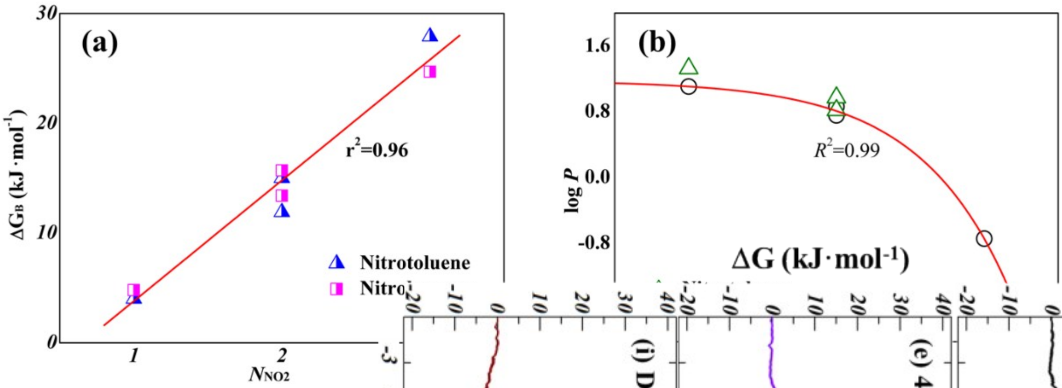

Figure S2. Correlation between (a ... NO$_2$ groups for selected explosives

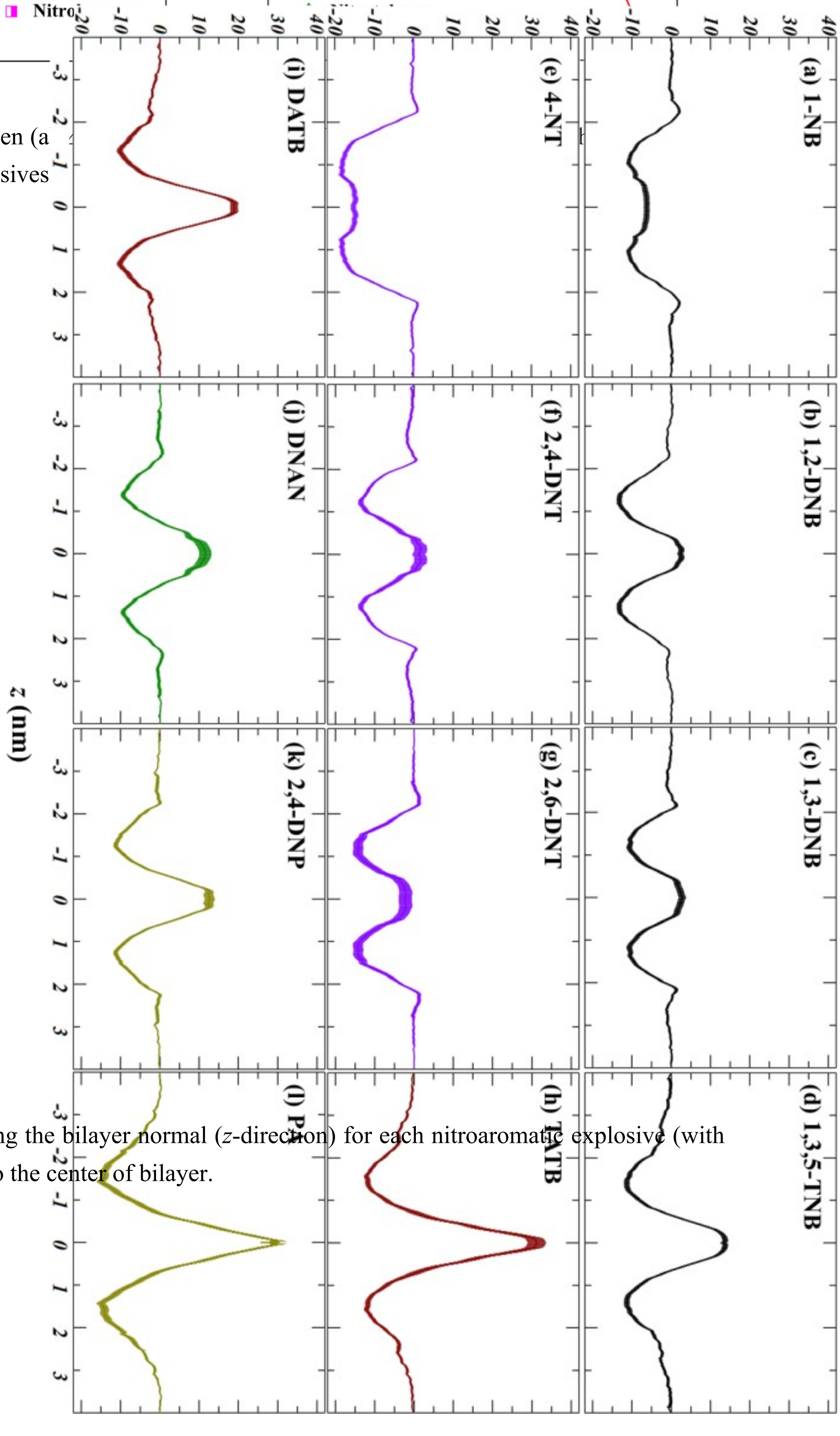

Figure S3. PMF profiles along the bilayer normal (z-direction) for each nitroaromatic explosive (with error bars). z=0 corresponds to the center of bilayer.

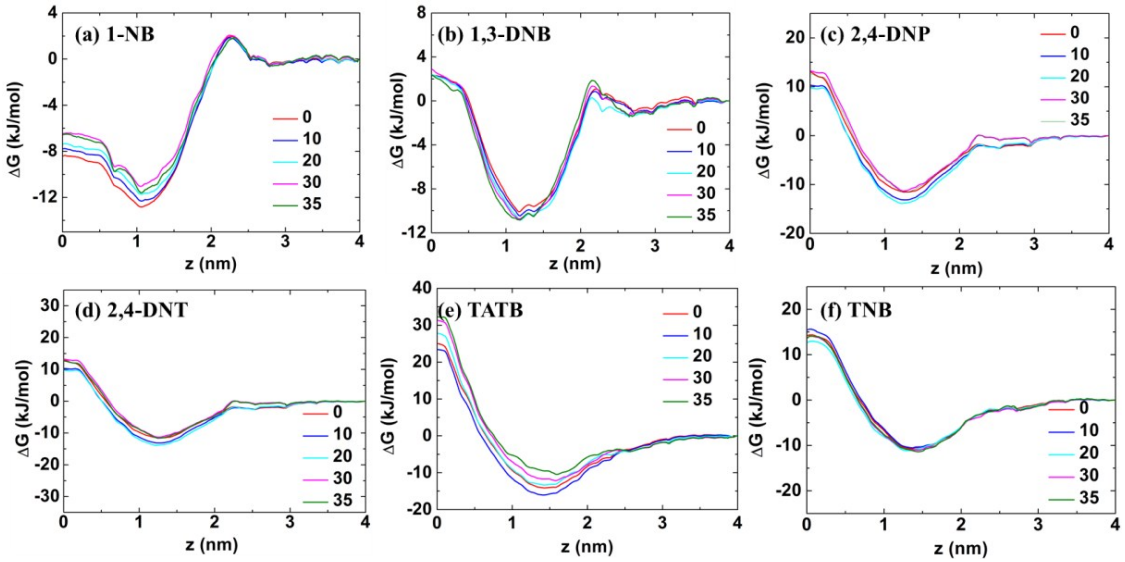

Figure S4. PMF profiles with different equilibration time. *z*=0 corresponds to the center of bilayer.