Figure S1. Scatter plots of collision cross sections vs. energy for 200 conformations sampled from MD simulations. a) 24:0-24:0 PC, b) 18:0-16:0 PC, and c) 16:0-22:6 PC

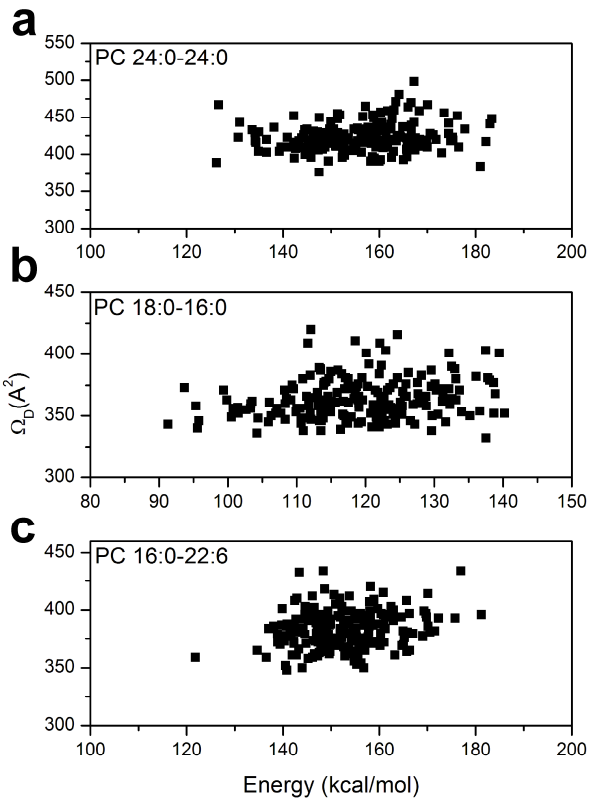
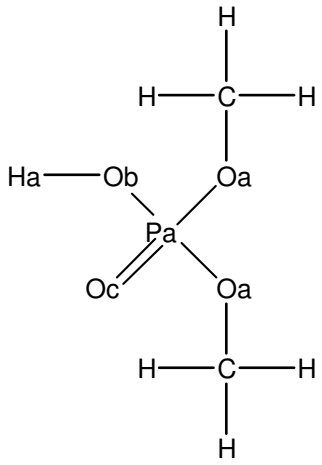


Table S1. Mass, drift time, and corrected drift time of ion molecule used in this study.

Name	cationization	[c]mass	t_d (ms)	[d]t_d'(ms)
[a]5:0-5:0 PC	H^+	426	3.58	3.39
	Na^+	448	3.97	3.77
[a]8:0-8:0 PC	H^+	510	4.99	4.78
	Na^+	532	5.50	5.29
[a]11:0-11:0 PC	H^+	594	6.40	6.18
	Na^+	616	6.85	6.62
[a]14:0-16:0 PC	H^+	706	8.06	7.82
	Na^+	728	8.32	8.07
[a]16:0-16:0 PC	H^+	734	8.64	8.39
	Na^+	756	8.77	8.51
[a]18:0-14:0 PC	H^+	734	8.58	8.33
	Na^+	756	8.77	8.51
[a,b]16:0-18:2 PC	H^+	758	8.51	8.26
[a]18:0-16:0 PC	H^+	762	8.96	8.71
	Na^+	784	9.15	8.89
[a]16:0-20:4 PC	H^+	782	8.58	8.32
[a,b]18:0-18:2 PC	H^+	786	8.90	8.64
[a]18:0-18:1 PC	H^+	788	8.96	8.70
[a]18:0-18:0 PC	H^+	790	9.41	9.15
[a]16:0-22:6 PC	H^+	806	8.83	8.57
[a]24:0-24:0 PC	H^+	958	12.2	11.9
[b]KK (cytC)	H^+	275	1.86	1.70
[b]HK (cytC)	H^+	284	1.86	1.70
[b]GKK (cytC)	H^+	332	2.37	2.20
[b]GGGGGG	H^+	362	2.18	2.00
[b]ATNE (cytC)	H^+	434	3.20	3.01
[b]AAAAAA	H^+	446	3.14	2.94
[b]KATNE (cytC)	H^+	563	4.29	4.07
[b]Ac-GDVEK (cytC)	H^+	590	4.80	4.58
[b]GITWK (cytC)	H^+	605	5.12	4.89
[b]IFVQK (cytC)	H^+	635	5.70	5.46
[b]YIPGTK (cytC)	H^+	679	6.02	5.78
[b]MIFAGIK (cytC)	H^+	780	7.36	7.10
[b]Bradykinin	H^+	1061	10.2	9.94
[b]TGPNLHGLFGR (cytC)	H^+	1169	11.8	11.5

[a]Molecules examined in this study. [b]Molecules used as calibrant. [c]All ions are singly charged. [d]Mass dependent corrected drift time.

Table S2. Optimized partial charge distribution of protonated phosphate from the DFT calculation of protonated dimethyl phosphate. The partial charges with atom types for CHARMM force field are tabulated.



	Mulliken Charge[a]	Force Field Charge	Force Field type
Pa	1.16	1.50	PL
Oa	-0.51	-0.49	OSL
Ob	-0.54	-0.52	OHL
Oc	-0.57	-0.56	O2L
Ha	0.35	0.36	HOL

[a]Computed from density functional theory (DFT) calculation using Jaguar 6.0 of Schroedinger company with B3LYP functional and 6-31G** basis set.

Table S3.

Name	[a]Mass	Applied Voltage (V)	t_d (ms)	[b]K_0 ($cm^2V^{-1}s^{-1}$)
8:0-8:0 PC	510	7	6.46	0.447
		7.5	5.504	0.453
		8	4.99	0.448
		8.5	4.16	0.463
14:0-16:0 PC	706	7	10.8	0.344
		7.5	9.28	0.347
		8	8.06	0.350
		8.5	7.04	0.353
18:0-18:0 PC	790	7	12.3	0.323
		7.5	10.6	0.324
		8	9.41	0.324
		8.5	8.16	0.328

[a]All ions are singly charged. [b]Evaluated using equations from Shavartsburg and Smith.[29]