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

Supplementary Information for

The potential mechanism of atmospheric new particle formation involving amino acids with multiple functional groups

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I. Boundary conditions.

II. Tables and Figures

Fig. S1 (a) The most stable configurations of (**SA**)$_2$·(**A**), and (**SA**)$_2$·(**A**)·(**ASP**) clusters. Hydrogen bonds are shown as dashed lines and the bond lengths are given in Å. (b) Relief map with the projection of localized orbital locator (LOL) of (**SA**)$_2$·(**A**), and (**SA**)$_2$·(**A**)·(**ASP**) clusters where LOL values are shown in the color map.

Fig. S2 (a) The most stable configurations of (**SA**)$_2$·(**A**)$_2$, and (**SA**)$_2$·(**A**)$_2$·(**ASP**) clusters. Hydrogen bonds are shown as dashed lines and the bond lengths are given in Å. (b) Relief map with the projection of localized orbital locator (LOL) of (**SA**)$_2$·(**A**)$_2$, and (**SA**)$_2$·(**A**)$_2$·(**ASP**) clusters where LOL values are shown in the color map.

Fig. S3 (a) The J (s^{-1}) and (b) R versus [**ASP**] with [**SA**] = 10^6 molecules cm^{-3}, [**A**] = 10^7 molecules cm^{-3} and four different temperatures (black line: 298 K, red line: 278 K, blue line: 258 K, green line: 238 K).

Fig. S4 (a) The J (s^{-1}) and (b) R versus [**ASP**] with [**SA**] = 10^8 molecules cm^{-3}, [**A**] = 10^{11} molecules cm^{-3} and four different temperatures (black line: 298 K, red line: 278 K, blue line: 258 K, green line: 238 K).

Fig. S5 (a) The J (s^{-1}) and (b) R versus of [**A**] with [**ASP**] = 10^6 molecules cm^{-3} and three different [**SA**] (red line: [**SA**] =10^6 molecules cm^{-3}, blue line: [**SA**] =10^7 molecules cm^{-3}, green line: [**SA**] = 10^8 molecules cm^{-3}) at 238 K.

Fig. S6 (a) The J (s^{-1}) and (b) R versus of [**A**] with [**ASP**] = 10^8 molecules cm^{-3} and three different [**SA**] (red line: [**SA**] = 10^6 molecules cm^{-3}, blue line: [**SA**] = 10^7 molecules cm^{-3}, green line: [**SA**] = 10^8 molecules cm^{-3}) at 238 K.

Fig. S7 ESP-mapped molecular vdW surface of (a) **ASP** and (b) **MOA** molecules. Surface local minima and maxima of ESP of the different functional groups in **ASP** and **MOA** molecules are represented as blue and yellow spheres, respectively.

Table S1 The Electron density ρ (a.u.), Laplacian Bond Order (LBO), bond distances r (Å) between the N and H atoms, Laplacian $\nabla^2 \rho$ (a.u.) at the BCPs, and the number of proton transfer N. The labeled atoms are corresponding to those shown in Figs. S1 and S2.

Table S2 Gibbs free energy of formation, ΔG (kcal mol^{-1}), for all clusters at pressure of 1 atm and temperatures of 298, 278, 258, and 238 K.

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III. Coordinates of the clusters in the system

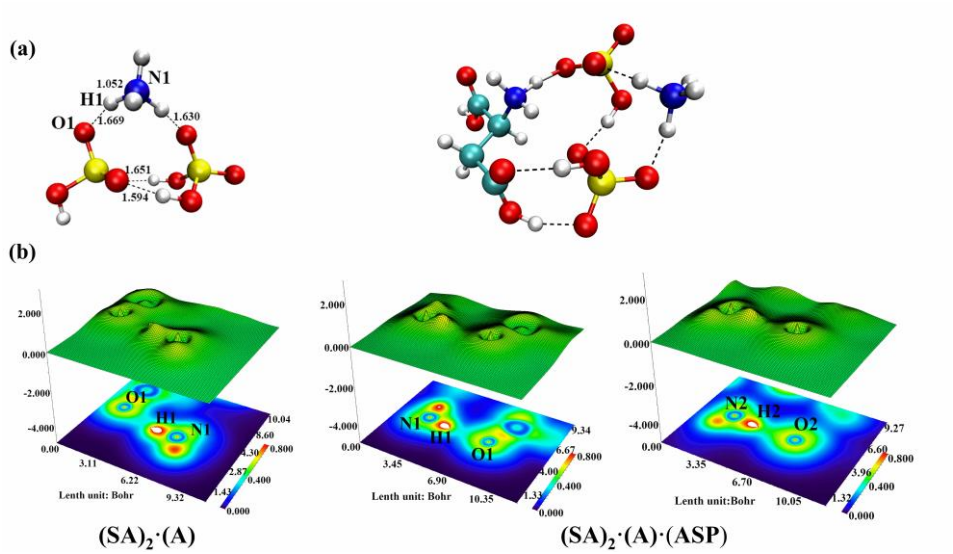
Tables S13 – S38. The XYZ coordinates of all the studied clusters.

I. Boundary conditions.

In the Atmospheric Cluster Dynamics Code (ACDC) simulations, some clusters growing out of the studied system are unstable and would evaporate back to smaller clusters, while others will continue to grow furtherly. Only clusters allowed to grow out of the studied system can be considered to contribute to the clusters' formation rate. Moreover, whether the cluster has the potential to grow out of the studied system depends on the boundary condition. In ACDC simulations, boundary condition refers to the smallest clusters out of the studied system, which are presumed to be stable enough to grow than evaporate back towards smaller sizes.

For the atmospheric new particle formation (NPF), the stability of the corresponding cluster could be determined by comparing the collision rate and evaporation rate. The collision rate further could be deduced by the collision rate coefficients and the concentration of the acid and base molecules. The results from the studied clusters show that the collision rate coefficients are on the same order of magnitude (10^{-9}~10^{-10} molecules^{-1} cm^3 s^{-1}). In the meantime, the evaporation rate chiefly depends on the formation Gibbs free energy of the clusters. Therefore, based on the above analyses, it can be found that the only cluster containing pure **SA** and **A** molecules as well as the cluster containing an **ASP** molecule except for **SA** and **A** molecules are relatively stable enough to resist evaporation and therefore can form larger clusters as well as contribute to particle formation rates. Hence, (**SA**)$_3$·(**A**)$_3$ and (**SA**)$_3$·**(A)**·(**ASP)** clusters are set to be boundary clusters at 238 K, respectively. The corresponding boundary conditions at different temperatures are also listed in Table S11. In addition, a constant coagulation sink coefficient 1×10^3 s^{-1} was used for considering external losses.

II. Tables and Figures



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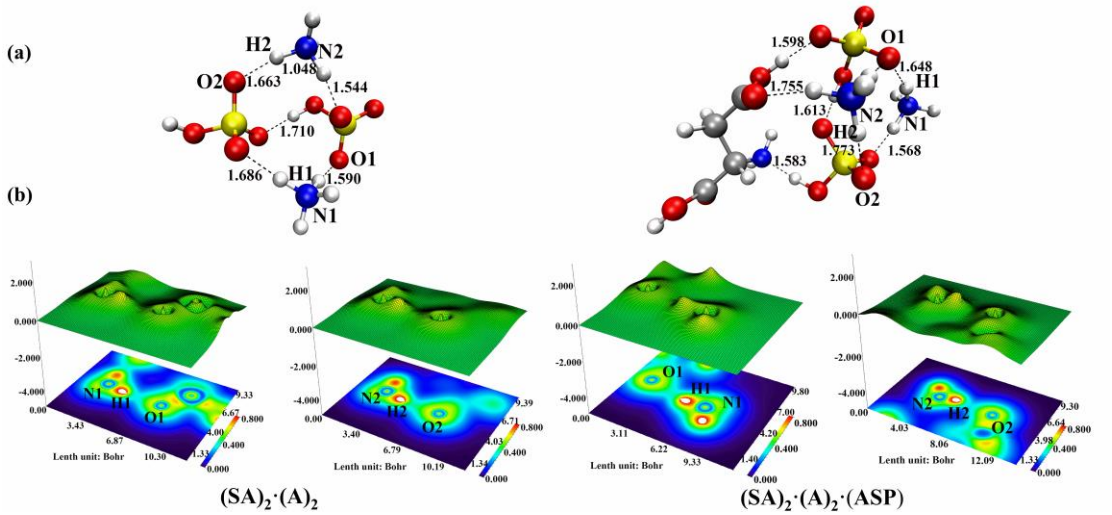

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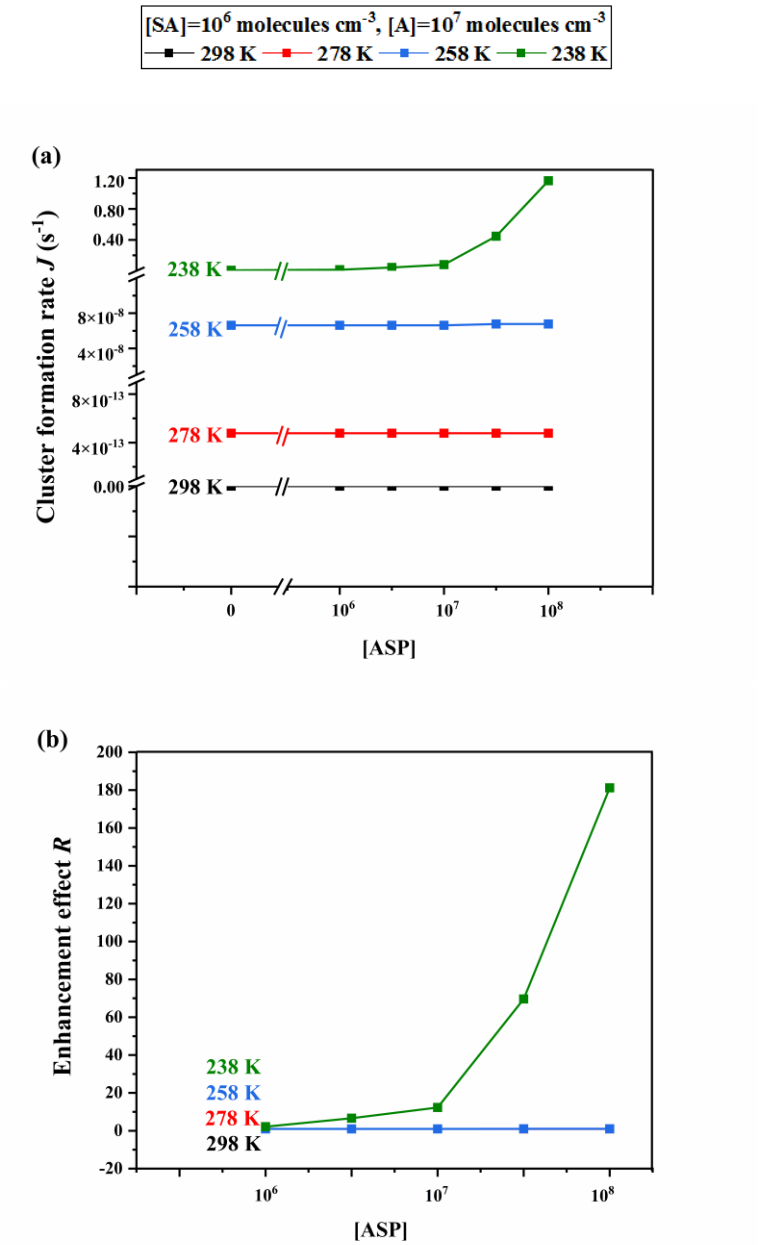

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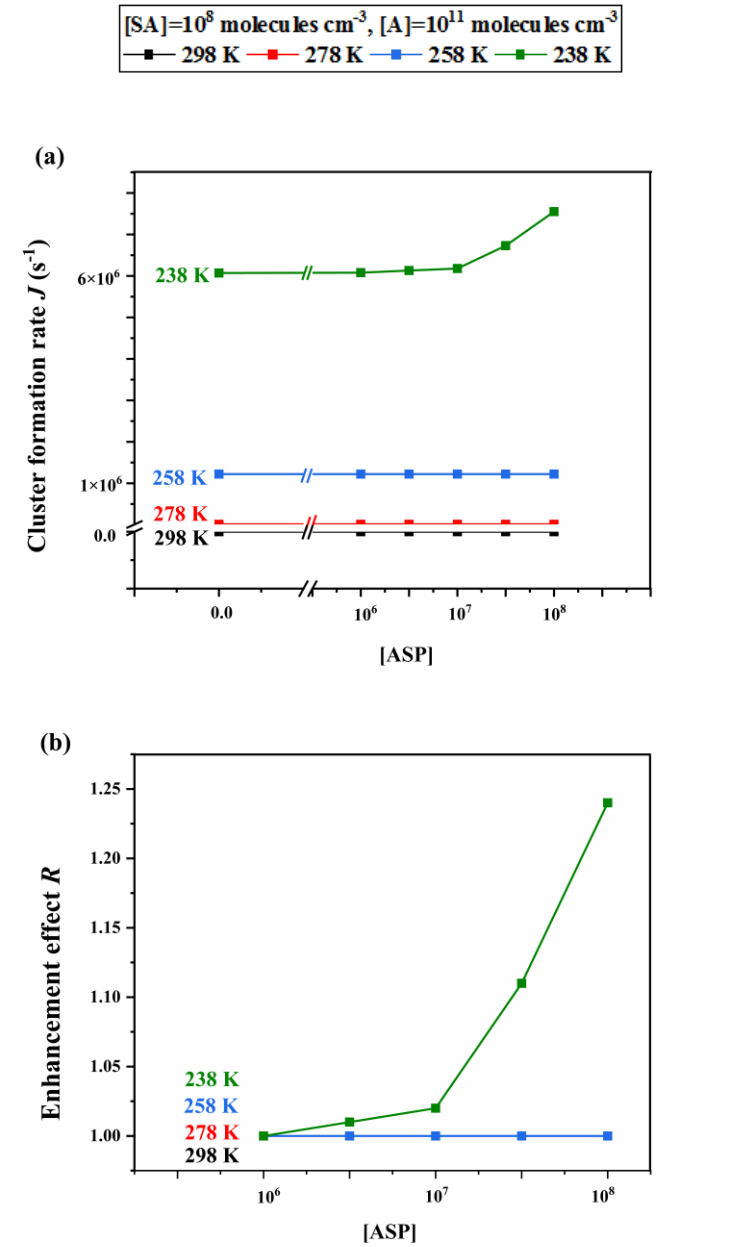

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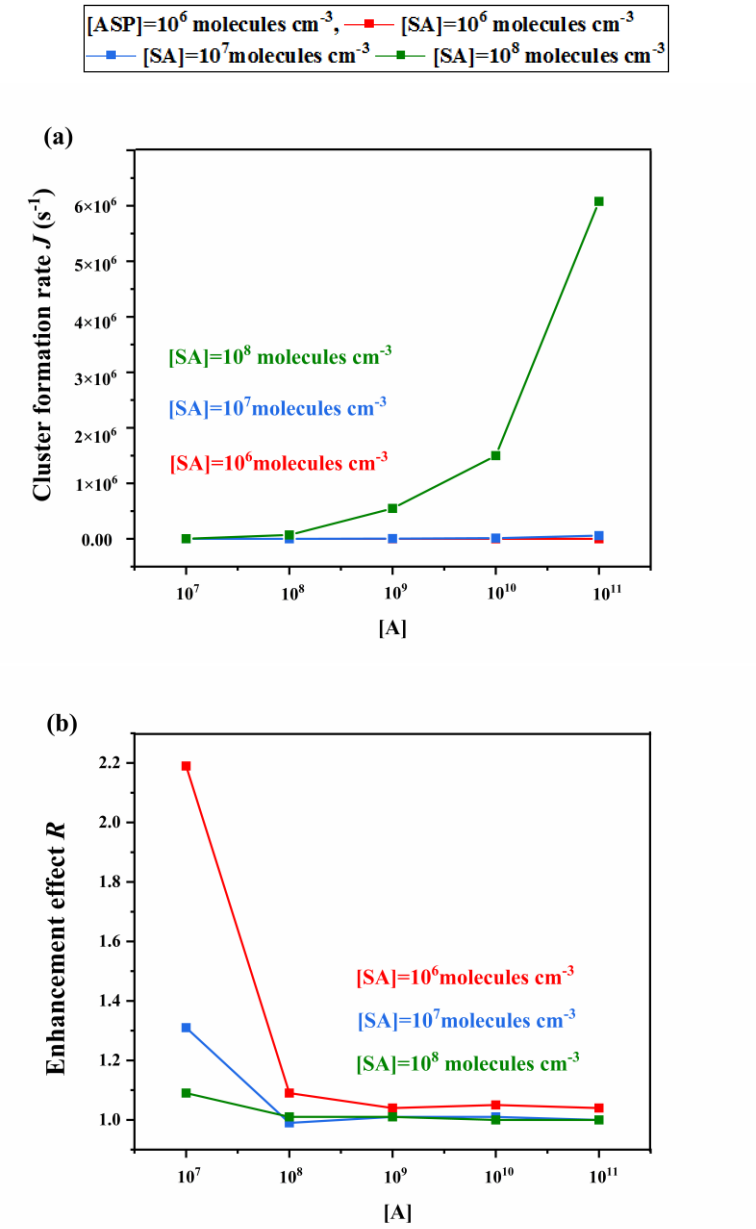

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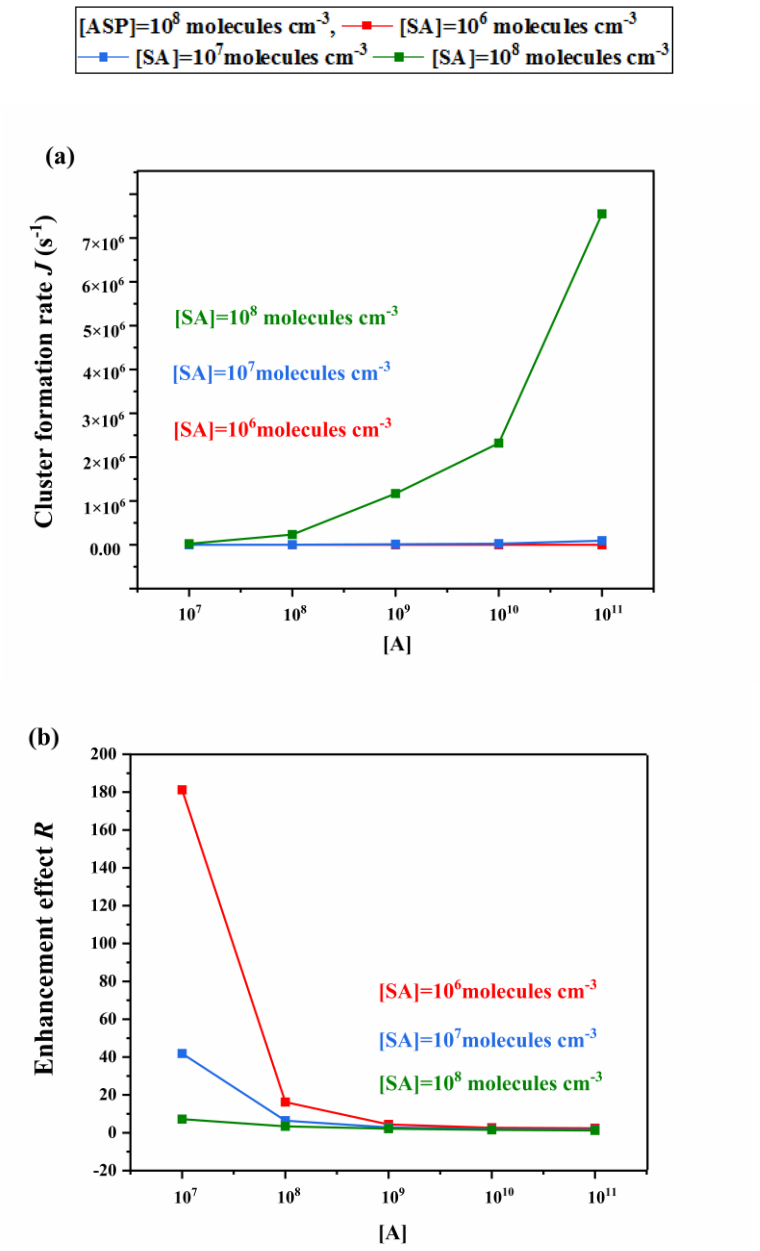

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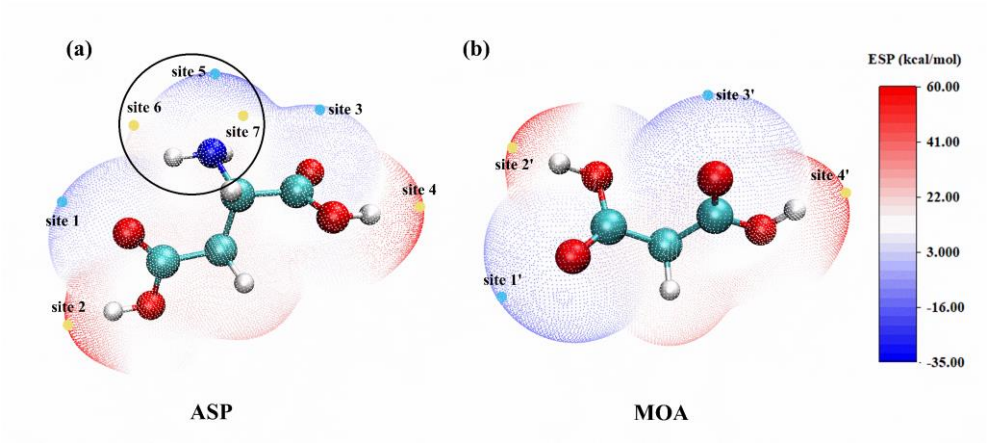

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Clusters	Bonds	ρ (a.u.)	LBO	r (Å)	$\nabla^2\rho$ (a.u.)	N
(SA)$_2$**·(A)**	N1-H1	0.3088	0.623	1.052	-1.864	1
(SA)$_2$**·(A)·(ASP)**	N1-H1	0.3256	0.683	1.048	-1.885	2
	N2-H2	0.2791	0.495	1.088	-1.596	
(SA)$_2$**·(A)**$_2$	N1-H1	0.3118	0.633	1.048	-1.880	2
	N2-H2	0.2945	0.570	1.067	-1.766	
(SA)$_2$**·(A)**$_2$**·(ASP)**	N1-H1	0.3241	0.682	1.032	-1.914	2
	N2-H2	0.3088	0.626	1.037	-1.816	

Table S2 Gibbs free energy of formation, ΔG (kcal mol^{-1}), for all clusters at pressure of 1 atm and temperatures of 298, 278, 258, and 238 K.

Clusters	238K	258K	278K	298K
(SA)$_2$	-10.45	-9.77	-9.10	-8.42
(SA)$_3$	-18.54	-17.00	-15.46	-13.91
(SA)·(A)	-9.15	-8.54	-7.94	-7.33
(SA)·(ASP)	-11.49	-10.62	-9.75	-8.87
(ASP)$_2$	-7.09	-6.34	-5.58	-4.82
(ASP)·(A)	-3.39	-2.75	-2.11	-1.47
(SA)$_2$**·(A)**	-25.52	-23.96	-22.41	-20.84
(SA)$_2$**·(ASP)**	-26.72	-24.93	-23.14	-21.35
(SA)·(ASP)$_2$	-23.45	-21.59	-19.73	-17.85
(ASP)$_2$**·(A)**	-8.51	-6.92	-5.33	-3.73
(SA)·(A)·(ASP)	-18.55	-17.04	-15.54	-14.03
(ASP)$_3$	-10.15	-5.69	-3.99	-2.28
(SA)$_3$**·(A)**	-37.17	-34.84	-32.52	-30.19
(SA)$_2$**·(A)**$_2$	-33.28	-31.04	-28.81	-26.56
(ASP)$_3$**·(A)**	-13.37	-8.23	-5.57	-2.90
(ASP)$_2$**·(A)**$_2$	-11.66	-9.39	-7.12	-4.89
(SA)$_2$**·(ASP)·(A)**	-38.48	-35.91	-33.33	-30.74
(SA)·(ASP)$_2$**·(A)**	-33.70	-31.05	-28.40	-25.73
(SA)·(ASP)·(A)$_2$	-20.12	-17.77	-15.42	-13.06
(SA)$_3$**·(A)**$_2$	-51.01	-47.94	-44.87	-41.79
(ASP)$_3$**·(A)**$_2$	-17.27	-13.85	-10.44	-7.00
(SA)$_2$**·(ASP)·(A)**$_2$	-49.84	-46.54	-43.24	-39.92
(SA)·(ASP)$_2$**·(A)**$_2$	-33.10	-29.79	-26.49	-23.17

Table S3 The enhancement strength (R) on cluster formation rate by **ASP** at all the monomers concentration (molecules cm^{-3}) conditions and T=238 K.

[**SA**]	[**A**]	[**ASP**]=10^6	[**ASP**]=5×10^6	[**ASP**]=10^7	[**ASP**]=5×10^7	[**ASP**]=10^8
[**SA**]=10^6	[**A**]=10^7	2.19	6.67	12.34	69.65	181.22
[**SA**]=10^6	[**A**]=10^8	1.09	1.46	1.95	6.82	16.26
[**SA**]=10^6	[**A**]=10^9	1.04	1.17	1.31	2.44	4.40
[**SA**]=10^6	[**A**]=10^{10}	1.05	1.17	1.26	1.76	2.64
[**SA**]=10^6	[**A**]=10^{11}	1.04	1.11	1.15	1.50	2.39
[**SA**]=10^7	[**A**]=10^7	1.31	2.46	3.91	17.79	41.88
[**SA**]=10^7	[**A**]=10^8	0.99	1.03	1.17	3.02	6.38
[**SA**]=10^7	[**A**]=10^9	1.01	1.07	1.14	1.77	2.86
[**SA**]=10^7	[**A**]=10^{10}	1.01	1.04	1.08	1.39	1.93
[**SA**]=10^7	[**A**]=10^{11}	1.00	1.02	1.04	1.24	1.65
[**SA**]=10^8	[**A**]=10^7	1.09	1.37	1.65	3.93	7.21
[**SA**]=10^8	[**A**]=10^8	1.01	1.06	1.14	2.00	3.39
[**SA**]=10^8	[**A**]=10^9	1.01	1.05	1.09	1.52	2.16
[**SA**]=10^8	[**A**]=10^{10}	1.00	1.02	1.04	1.24	1.55
[**SA**]=10^8	[**A**]=10^{11}	1.00	1.01	1.02	1.11	1.24

Table S4 The enhancement strength (R) on cluster formation rate by **ASP** at all the monomers concentration (molecules cm^{-3}) conditions and T=258 K.

[**SA**]	[**A**]	[**ASP**]=10^6	[**ASP**]=5×10^6	[**ASP**]=10^7	[**ASP**]=5×10^7	[**ASP**]=10^8
[**SA**]=10^6	[**A**]=10^7	1.00	1.00	1.00	1.02	1.02
[**SA**]=10^6	[**A**]=10^8	1.00	1.00	1.00	1.03	1.02
[**SA**]=10^6	[**A**]=10^9	1.00	1.00	1.01	1.04	1.08
[**SA**]=10^6	[**A**]=10^{10}	1.00	1.01	1.01	1.05	1.02
[**SA**]=10^6	[**A**]=10^{11}	1.00	1.01	1.03	1.14	1.02
[**SA**]=10^7	[**A**]=10^7	0.99	0.98	0.96	0.90	1.02
[**SA**]=10^7	[**A**]=10^8	1.00	0.98	0.97	0.92	1.02
[**SA**]=10^7	[**A**]=10^9	1.00	1.00	1.00	1.00	1.02
[**SA**]=10^7	[**A**]=10^{10}	1.00	1.00	1.01	1.05	1.02
[**SA**]=10^7	[**A**]=10^{11}	1.00	1.01	1.02	1.08	1.02
[**SA**]=10^8	[**A**]=10^7	0.98	0.90	0.83	0.56	1.02
[**SA**]=10^8	[**A**]=10^8	0.98	0.92	0.85	0.59	1.02
[**SA**]=10^8	[**A**]=10^9	0.99	0.97	0.94	0.79	1.04
[**SA**]=10^8	[**A**]=10^{10}	1.00	1.00	1.00	1.01	1.04
[**SA**]=10^8	[**A**]=10^{11}	1.00	1.00	1.00	1.02	1.02

Table S5 The enhancement strength (R) on cluster formation rate by **ASP** at all the monomers concentration (molecules cm^{-3}) conditions and T=278 K.

[**SA**]	[**A**]	[**ASP**]=10^6	[**ASP**]=5×10^6	[**ASP**]=10^7	[**ASP**]=5×10^7	[**ASP**]=10^8
[**SA**]=10^6	[**A**]=10^7	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^6	[**A**]=10^8	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^6	[**A**]=10^9	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^6	[**A**]=10^{10}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^6	[**A**]=10^{11}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^7	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^8	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^9	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^{10}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^{11}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^7	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^8	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^9	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^{10}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^{11}	1.00	1.00	1.00	1.00	1.00

Table S6 The enhancement strength (R) on cluster formation rate by **ASP** at all the monomers concentration (molecules cm^{-3}) conditions and T=298 K.

[**SA**]	[**A**]	[**ASP**]=10^6	[**ASP**]=5×10^6	[**ASP**]=10^7	[**ASP**]= 5×10^7	[**ASP**]=10^8
[**SA**]=10^6	[**A**]=10^7	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^6	[**A**]=10^8	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^6	[**A**]=10^9	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^6	[**A**]=10^{10}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^6	[**A**]=10^{11}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^7	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^8	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^9	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^{10}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^7	[**A**]=10^{11}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^7	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^8	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^9	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^{10}	1.00	1.00	1.00	1.00	1.00
[**SA**]=10^8	[**A**]=10^{11}	1.00	1.00	1.00	1.00	1.00

Table S7 Evaporation rate coefficients (s^{-1}) of monomer from corresponding clusters in the system at T = 238 K.

Clusters	Evaporation rate coefficients	Clusters	Evaporation rate coefficients
2SA→1SA+1SA	1.23	**2ASP·2A→2ASP·1A+1A**	6.04×10^{7}
1SA·1A→1SA+1A	5.01×10^{1}	**2SA·1ASP·1A→1SA·1ASP·1A +1SA**	8.78×10^{-9}
1SA·ASP→1SA+1ASP	4.37×10^{-1}	**2SA·1ASP·1A→2SA·1ASP+1A**	4.45×10^{-1}
1ASP·1A→1ASP +1A	1.79×10^{7}	**2SA·1ASP·1A→1SA·1A+1ASP**	2.58×10^{-2}
2ASP→1ASP+1ASP	3.38×10^{3}	**1SA·2ASP·1A→2ASP·1A+1SA**	1.96×10^{-13}
3SA→2SA+1SA	5.40×10^{2}	**1SA·2ASP·1A→1SA·2ASP+1A**	1.80×10^{1}
2SA·1A→2SA+1A	3.33×10^{-4}	**1SA·2ASP·1A→1SA·1ASP·1A+1ASP**	2.85×10^{-4}
2SA·1A→1SA·1A+1SA	1.25×10^{-5}	**1SA·1ASP·2A→1SA·1ASP·1A+1A**	1.06×10^{9}
3ASP→2ASP+1ASP	5.45×10^{7}	**3SA·2A→2SA·2A+1SA**	8.44×10^{-7}
1SA·2ASP→2ASP+1SA	2.74×10^{-5}	**3SA·2A→3SA·1A+1A**	5.11×10^{-3}
1SA·2ASP→1SA·1ASP+1ASP	2.63×10^{-1}	**3ASP·2A→2ASP·2A+1ASP**	1.90×10^{5}
2ASP·1A→2ASP+1A	2.55×10^{9}	**3ASP·2A→3ASP·1A+1A**	1.43×10^{7}
2ASP·1A→1ASP·1A+1ASP	2.34×10^{5}	**2SA·1ASP·2A→1SA·1ASP·2A+1SA**	9.07×10^{-18}
1SA·1ASP·1A→1ASP·1A+1SA	2.41×10^{-4}	**2SA·1ASP·2A→2SA·2A+1ASP**	1.35×10^{-5}
1SA·1ASP·1A→1SA·1ASP+1A	1.07×10^{4}	**2SA·1ASP·2A→2SA·1ASP·1A+1A**	1.25
1SA·1ASP·1A→1SA·1A+1ASP	4.60×10^{1}	**1SA·2ASP·2A→2ASP·2A+1SA**	4.37×10^{-10}
2SA·ASP→SA·ASP +1SA	2.01×10^{-4}	**1SA·2ASP·2A→1SA·2ASP·1A+1A**	1.36×10^{11}
2SA·ASP→2SA +1ASP	2.31×10^{-5}	**1SA·2ASP·2A→1SA·1ASP·2A+1ASP**	2.81×10^{-2}
3SA·1A→2SA·1A+1SA	3.00×10^{-1}	**2SA·2A→2SA·1A+1A**	1.80×10^{3}
3SA·1A→3SA+1A	2.37×10^{-7}	**3ASP·1A→3ASP+1A**	6.10×10^{7}
3ASP·1A→2ASP·1A+1ASP	1.12×10^{6}		

Table S8 Evaporation rate coefficients (s^{-1}) of monomer from corresponding clusters in the system at T = 258 K.

Clusters	Evaporation rate coefficients	Clusters	Evaporation rate coefficients
2**SA**→1**SA**+1**SA**	2.46×10^{1}	2**ASP**·2**A**→2**ASP**·1**A**+1**A**	3.67×10^{8}
1**SA**·1**A**→1**SA**+1**A**	7.09×10^{2}	2**SA**·1**ASP**·1**A**→1**SA**·1**ASP**·1**A** +1**SA**	1.75×10^{-6}
1**SA**·**ASP**→1**SA**+1**ASP**	1.50×10^{1}	2**SA**·1**ASP**·1**A**→2**SA**·1**ASP**+1**A**	1.34×10^{1}
1**ASP**·1**A**→1**ASP** +1**A**	1.05×10^{8}	2**SA**·1**ASP**·1**A**→1**SA**·1**A**+1**ASP**	1.49
2**ASP**→1**ASP**+1**ASP**	4.47×10^{4}	1**SA**·2**ASP**·1**A**→2**ASP**·1**A**+1**SA**	9.24×10^{-11}
3**SA**→2**SA**+1**SA**	1.05×10^{4}	1**SA**·2**ASP**·1**A**→1**SA**·2**ASP**+1**A**	4.32×10^{2}
2**SA**·1**A**→2**SA**+1**A**	2.11×10^{-2}	1**SA**·2**ASP**·1**A**→1**SA**·1**ASP**·1**A**+1**ASP**	3.02×10^{-2}
2**SA**·1**A**→1**SA**·1**A**+1**SA**	1.12×10^{-3}	1**SA**·1**ASP**·2**A**→1**SA**·1**ASP**·1**A**+1**A**	6.81×10^{9}
3**ASP**→2**ASP**+1**ASP**	1.20×10^{11}	3**SA**·2**A**→2**SA**·2**A**+1**SA**	7.48×10^{-5}
1**SA**·2**ASP**→2**ASP**+1**SA**	3.35×10^{-3}	3**SA**·2**A**→3**SA**·1**A**+1**A**	2.02×10^{-1}
1**SA**·2**ASP**→1**SA**·1**ASP**+1**ASP**	1.24×10^{1}	3**ASP**·2**A**→2**ASP**·2**A**+1**ASP**	4.31×10^{6}
2**ASP**·1**A**→2**ASP**+1**A**	1.59×10^{10}	3**ASP**·2**A**→3**ASP**·1**A**+1**A**	9.11×10^{5}
2**ASP**·1**A**→1**ASP**·1**A**+1**ASP**	7.57×10^{6}	2**SA**·1**ASP**·2**A**→1**SA**·1**ASP**·2**A**+1**SA**	7.25×10^{-15}
1**SA**·1**ASP**·1**A**→1**ASP**·1**A**+1**SA**	1.52×10^{-2}	2**SA**·1**ASP**·2**A**→2**SA**·2**A**+1**ASP**	1.55×10^{-3}
1**SA**·1**ASP**·1**A**→1**SA**·1**ASP**+1**A**	1.14×10^{5}	2**SA**·1**ASP**·2**A**→2**SA**·1**ASP**·1**A**+1**A**	3.22×10^{1}
1**SA**·1**ASP**·1**A**→1**SA**·1**A**+1**ASP**	1.19×10^{3}	1**SA**·2**ASP**·2**A**→2**ASP**·2**A**+1**SA**	1.07×10^{-7}
2**SA**·**ASP**→**SA**·**ASP** +1**SA**	1.41×10^{-2}	1**SA**·2**ASP**·2**A**→1**SA**·2**ASP**·1**A**+1**A**	4.28×10^{11}
2**SA**·**ASP**→2**SA** +1**ASP**	2.79×10^{-3}	1**SA**·2**ASP**·2**A**→1**SA**·1**ASP**·2**A**+1**ASP**	1.47
3**SA**·1**A**→2**SA**·1**A**+1**SA**	8.72	2**SA**·2**A**→2**SA**·1**A**+1**A**	2.32×10^{4}
3**SA**·1**A**→3**SA**+1**A**	2.25×10^{-5}	3**ASP**·1**A**→3**ASP**+1**A**	3.74×10^{8}
3**ASP**·1**A**→2**ASP**·1**A**+1**ASP**	2.43×10^{9}		

Table S9 Evaporation rate coefficients (s^{-1}) of monomer from corresponding clusters in the system at T = 278 K.

Clusters	Evaporation rate coefficients	Clusters	Evaporation rate coefficients
2**SA**→1**SA**+1**SA**	3.14×10^{2}	2**ASP**·2**A**→2**ASP**·1**A**+1**A**	1.71×10^{9}
1**SA**·1**A**→1**SA**+1**A**	6.70×10^{3}	2**SA**·1**ASP**·1**A**→1**SA**·1**ASP**·1**A** +1**SA**	1.68×10^{-4}
1**SA**·**ASP**→1**SA**+1**ASP**	3.11×10^{2}	2**SA**·1**ASP**·1**A**→2**SA**·1**ASP**+1**A**	2.52×10^{2}
1**ASP**·1**A**→1**ASP** +1**A**	4.72×10^{8}	2**SA**·1**ASP**·1**A**→1**SA**·1**A**+1**ASP**	4.94×10^{1}
2**ASP**→1**ASP**+1**ASP**	4.16×10^{5}	1**SA**·2**ASP**·1**A**→2**ASP**·1**A**+1**SA**	1.79×10^{-8}
3**SA**→2**SA**+1**SA**	1.34×10^{5}	1**SA**·2**ASP**·1**A**→1**SA**·2**ASP**+1**A**	6.56×10^{3}
2**SA**·1**A**→2**SA**+1**A**	7.31×10^{-1}	1**SA**·2**ASP**·1**A**→1**SA**·1**ASP**·1**A**+1**ASP**	1.67
2**SA**·1**A**→1**SA**·1**A**+1**SA**	5.23×10^{-2}	1**SA**·1**ASP**·2**A**→1**SA**·1**ASP**·1**A**+1**A**	3.39×10^{10}
3**ASP**→2**ASP**+1**ASP**	5.79×10^{11}	3**SA**·2**A**→2**SA**·2**A**+1**SA**	3.53×10^{-3}
1**SA**·2**ASP**→2**ASP**+1**SA**	2.01×10^{-1}	3**SA**·2**A**→3**SA**·1**A**+1**A**	4.73
1**SA**·2**ASP**→1**SA**·1**ASP**+1**ASP**	3.34×10^{2}	3**ASP**·2**A**→2**ASP**·2**A**+1**ASP**	6.12×10^{7}
2**ASP**·1**A**→2**ASP**+1**A**	7.48×10^{10}	3**ASP**·2**A**→3**ASP**·1**A**+1**A**	7.51×10^{6}
2**ASP**·1**A**→1**ASP**·1**A**+1**ASP**	7.31×10^{7}	2**SA**·1**ASP**·2**A**→1**SA**·1**ASP**·2**A**+1**SA**	2.21×10^{-12}
1**SA**·1**ASP**·1**A**→1**ASP**·1**A**+1**SA**	5.15×10^{-1}	2**SA**·1**ASP**·2**A**→2**SA**·2**A**+1**ASP**	9.11×10^{-2}
1**SA**·1**ASP**·1**A**→1**SA**·1**ASP**+1**A**	8.46×10^{5}	2**SA**·1**ASP**·2**A**→2**SA**·1**ASP**·1**A**+1**A**	5.08×10^{2}
1**SA**·1**ASP**·1**A**→1**SA**·1**A**+1**ASP**	1.93×10^{4}	1**SA**·2**ASP**·2**A**→2**ASP**·2**A**+1**SA**	1.16×10^{-5}
2**SA**·**ASP**→**SA**·**ASP** +1**SA**	5.34×10^{-1}	1**SA**·2**ASP**·2**A**→1**SA**·2**ASP**·1**A**+1**A**	1.12×10^{12}
2**SA**·**ASP**→2**SA** +1**ASP**	1.71×10^{-1}	1**SA**·2**ASP**·2**A**→1**SA**·1**ASP**·2**A**+1**ASP**	4.27×10^{1}
3**SA**·1**A**→2**SA**·1**A**+1**SA**	1.56×10^{2}	2**SA**·2**A**→2**SA**·1**A**+1**A**	2.07×10^{5}
3**SA**·1**A**→3**SA**+1**A**	1.09×10^{-3}	3**ASP**·1**A**→3**ASP**+1**A**	2.93×10^{9}
3**ASP**·1**A**→2**ASP**·1**A**+1**ASP**	1.95×10^{10}		

Table S10 Evaporation rate coefficients (s^{-1}) of monomer from corresponding clusters in the system at T = 298 K.

Clusters	Evaporation rate coefficients	Clusters	Evaporation rate coefficients
2**SA**→1**SA**+1**SA**	2.89×10^{3}	2**ASP**·2**A**→2**ASP**·1**A**+1**A**	5.94×10^{9}
1**SA**·1**A**→1**SA**+1**A**	4.76×10^{4}	2**SA**·1**ASP**·1**A**→1**SA**·1**ASP**·1**A** +1**SA**	8.73×10^{-3}
1**SA**·**ASP**→1**SA**+1**ASP**	4.34×10^{3}	2**SA**·1**ASP**·1**A**→2**SA**·1**ASP**+1**A**	3.25×10^{3}
1**ASP**·1**A**→1**ASP** +1**A**	1.74×10^{9}	2**SA**·1**ASP**·1**A**→1**SA**·1**A**+1**ASP**	1.01×10^{3}
2**ASP**→1**ASP**+1**ASP**	2.86×10^{6}	1**SA**·2**ASP**·1**A**→2**ASP**·1**A**+1**SA**	1.74×10^{-6}
3**SA**→2**SA**+1**SA**	1.22×10^{6}	1**SA**·2**ASP**·1**A**→1**SA**·2**ASP**+1**A**	6.89×10^{4}
2**SA**·1**A**→2**SA**+1**A**	1.60×10^{1}	1**SA**·2**ASP**·1**A**→1**SA**·1**ASP**·1**A**+1**ASP**	5.45×10^{1}
2**SA**·1**A**→1**SA**·1**A**+1**SA**	1.48	1**SA**·1**ASP**·2**A**→1**SA**·1**ASP**·1**A**+1**A**	1.35×10^{11}
3**ASP**→2**ASP**+1**ASP**	2.29×10^{12}	3**SA**·2**A**→2**SA**·2**A**+1**SA**	9.75×10^{-2}
1**SA**·2**ASP**→2**ASP**+1**SA**	7.17	3**SA**·2**A**→3**SA**·1**A**+1**A**	7.26×10^{1}
1**SA**·2**ASP**→1**SA**·1**ASP**+1**ASP**	5.86×10^{3}	3**ASP**·2**A**→2**ASP**·2**A**+1**ASP**	6.83×10^{8}
2**ASP**·1**A**→2**ASP**+1**A**	2.90×10^{11}	3**ASP**·2**A**→3**ASP**·1**A**+1**A**	4.81×10^{7}
2**ASP**·1**A**→1**ASP**·1**A**+1**ASP**	5.28×10^{8}	2**SA**·1**ASP**·2**A**→1**SA**·1**ASP**·2**A**+1**SA**	3.17×10^{-10}
1**SA**·1**ASP**·1**A**→1**ASP**·1**A**+1**SA**	1.11×10^{1}	2**SA**·1**ASP**·2**A**→2**SA**·2**A**+1**ASP**	3.09
1**SA**·1**ASP**·1**A**→1**SA**·1**ASP**+1**A**	4.79×10^{6}	2**SA**·1**ASP**·2**A**→2**SA**·1**ASP**·1**A**+1**A**	5.61×10^{3}
1**SA**·1**ASP**·1**A**→1**SA**·1**A**+1**ASP**	2.15×10^{5}	1**SA**·2**ASP**·2**A**→2**ASP**·2**A**+1**SA**	7.46×10^{-4}
2**SA**·**ASP**→**SA**·**ASP** +1**SA**	1.22×10^{1}	1**SA**·2**ASP**·2**A**→1**SA**·2**ASP**·1**A**+1**A**	2.57×10^{12}
2**SA**·**ASP**→2**SA** +1**ASP**	5.92	1**SA**·2**ASP**·2**A**→1**SA**·1**ASP**·1**A**+1**ASP**	8.01×10^{2}
3**SA**·1**A**→2**SA**·1**A**+1**SA**	1.85×10^{3}	2**SA**·2**A**→2**SA**·1**A**+1**A**	1.37×10^{6}
3**SA**·1**A**→3**SA**+1**A**	3.12×10^{-2}	3**ASP**·1**A**→3**ASP**+1**A**	1.73×10^{10}
3**ASP**·1**A**→2**ASP**·1**A**+1**ASP**	1.18×10^{11}		

Table S11 Boundary condition at 298K, 278 K, 258K and 238 K, respectively.

Temperature	Boundary clusters
298K	$(\mathbf{SA})_3 \cdot (\mathbf{A})_3$
278K	$(\mathbf{SA})_3 \cdot (\mathbf{A})_3$
258K	$(\mathbf{SA})_3 \cdot (\mathbf{A})_3$
238K	$(\mathbf{SA})_3 \cdot (\mathbf{A})_3$, $(\mathbf{SA})_3 \cdot \mathbf{(A)} \cdot (\mathbf{ASP})$

Table S12 The values of surface local minima and maxima of ESP of the different functional groups in **ASP** and **MOA** molecules. The labeled site numbers are corresponding to those shown in Fig. S7.

Molecules	Functional groups	Site numbers	ESP (kcal/mol)
ASP	-COOH	1	56.17
		2	-26.04
	-COOH	3	-26.04
		4	56.17
	$-NH_2$	5	-34.71
		6	20.96
		7	20.96
MOA	-COOH	1’	56.71
		2’	-29.85
	-COOH	3’	56.71
		4’	-29.85

III. Coordinates of the clusters in the system

Table S13. Coordinates of **SA**. Units are in angstrom.

Atom	X	Y	Z
S	-0.000002	0.000001	-0.153840
O	0.641015	-1.068244	-0.819725
O	-0.641020	1.068270	-0.819690
O	1.029516	0.662937	0.836058
O	-1.029509	-0.662963	0.836045
H	1.691785	0.010654	1.099951
H	-1.691765	-0.010681	1.099974

Table S14. Coordinates of **A**. Units are in angstrom.

Atom	X	Y	Z
N	0.000000	0.113488	0.000000
H	-0.939049	-0.264998	0.000000
H	0.469524	-0.264710	0.813353

Table S15. Coordinates of **ASP**. Units are in angstrom.

Atom	X	Y	Z
C	-0.510929	0.385494	-0.354267
H	-0.371751	0.310722	-1.432717
N	-0.453859	1.772637	0.039483
H	-0.787484	1.892300	0.987989
H	0.487075	2.130649	-0.050557
C	-1.881844	-0.157951	-0.012957
O	-2.583063	0.260784	0.860556
O	-2.203590	-1.222219	-0.765768
H	-3.061773	-1.545080	-0.461082
C	0.509869	-0.542762	0.325069
H	0.361511	-1.584345	0.032988
H	0.405111	-0.496933	1.411073
O	2.816285	-0.941030	0.606026
C	1.923704	-0.167112	-0.029468
O	2.245626	0.706400	-0.784276

Table S16. Coordinates of $(\mathbf{SA})_2$. Units are in angstrom.

Atom	X	Y	Z
S	-2.035487	-0.073173	0.114174
O	-1.067162	0.084496	1.156741

O	-3.311024	-0.603152	0.396130
O	-2.180636	1.369567	-0.491854
H	-2.959535	1.415304	-1.063055
O	-1.423669	-0.890222	-1.038406
H	-0.462450	-0.657408	-1.157871
O	1.067111	-0.085041	-1.156651
S	2.035447	0.073169	-0.114181
O	1.423398	0.890156	1.038314
O	3.310760	0.603600	-0.396318
O	2.181233	-1.369418	0.492059
H	0.462240	0.657071	1.157837
H	2.960289	-1.414778	1.063076

Table S17. Coordinates of (**SA**)·(**A**). Units are in angstrom.

Atom	X	Y	Z
S	-0.598705	-0.112567	0.085247
O	0.102650	-0.107436	1.324258
O	-1.757163	-0.906227	-0.109555
O	0.387982	-0.388929	-1.057132
O	-1.008722	1.400070	-0.155160
H	1.367683	-0.203478	-0.740440
H	-1.744008	1.429702	-0.779557
N	2.731959	0.043275	-0.051253
H	3.195629	0.914291	-0.278558
H	3.405900	-0.706706	-0.145097
H	2.432383	0.084523	0.919177

Table S18. Coordinates of (**SA**)·(**ASP**). Units are in angstrom.

Atom	X	Y	Z
C	-1.120251	0.194716	-0.019924
H	-0.920966	-0.199425	-1.015962
N	-0.674219	-0.790033	0.959173
H	-0.730628	-0.406960	1.898069
H	-1.272569	-1.607936	0.897529
C	-0.282498	1.445253	0.134282
O	0.429508	1.670080	1.080373
O	-0.476334	2.298317	-0.859919
H	0.108803	3.057446	-0.735199
C	-2.599939	0.577586	0.086388
H	-2.852568	1.350860	-0.638883
H	-2.831245	0.983610	1.074394
O	-4.790686	-0.250875	-0.157832
C	-3.502096	-0.605392	-0.152880
O	-3.132935	-1.734999	-0.314708

H	-5.317470	-1.047506	-0.307808
S	2.598240	-0.472824	-0.252561
O	3.789496	-1.049496	-0.738744
O	1.645910	0.113600	-1.149774
O	1.861490	-1.506574	0.624752
H	0.877937	-1.245358	0.743240
O	3.031924	0.634064	0.775554
H	2.248113	1.144763	1.046570

Table S19. Coordinates of (**ASP**)·(**A**). Units are in angstrom.

Atom	X	Y	Z
C	-1.141336	0.379450	-0.344452
H	-0.957311	0.298936	-1.415591
N	-1.080277	1.769664	0.045565
H	-1.449887	1.892795	0.980511
H	-0.125560	2.099737	0.002909
C	-2.532473	-0.140890	-0.059805
O	-3.263218	0.286961	0.785648
O	-2.844060	-1.199077	-0.826886
H	-3.717036	-1.507696	-0.551601
C	-0.162007	-0.556753	0.380717
H	-0.316971	-1.598181	0.091912
H	-0.310378	-0.500356	1.461051
O	2.126282	-0.976060	0.7436690
C	1.277499	-0.211760	0.082464
O	1.612580	0.664743	-0.681050
H	3.062115	-0.705580	0.500436
N	4.498794	-0.002718	-0.135121
H	5.088817	0.536970	0.485876
H	3.991251	0.645938	-0.730317
H	5.102566	-0.564005	-0.722886

Table S20. Coordinates of (**ASP**)$_2$. Units are in angstrom.

Atom	X	Y	Z
C	-4.068018	0.439885	0.409068
H	-3.641550	1.441800	0.454592
N	-4.059898	-0.143846	1.729302
H	-4.643762	-0.970750	1.760802
H	-3.118166	-0.369543	2.018007
C	-5.503609	0.556530	-0.056766
O	-6.398365	-0.146939	0.309985
O	-5.653317	1.508438	-0.991597
H	-6.574988	1.489899	-1.281036
C	-3.319343	-0.352944	-0.674422

H	-3.437000	0.106228	-1.658552
H	-3.712637	-1.368558	-0.748610
O	-1.204613	-1.201615	-1.252521
C	-1.841791	-0.441460	-0.403097
O	-1.303122	0.151974	0.516579
H	-0.226221	-1.216651	-1.047546
C	3.407233	-0.615098	0.382554
H	3.614818	-0.602445	1.452108
N	3.957352	-1.818926	-0.193075
H	3.642332	-1.942241	-1.147256
H	4.967585	-1.794818	-0.161088
C	1.905962	-0.612227	0.200233
O	1.366340	-1.197920	-0.719899
O	1.272380	0.124573	1.075659
H	0.295531	0.142269	0.873801
C	3.918649	0.706001	-0.217288
H	3.408050	1.567082	0.218789
H	3.736737	0.735982	-1.293477
O	5.857682	1.999629	-0.564016
C	5.394440	0.885038	0.019925
O	6.093584	0.144850	0.652174
H	6.801404	2.062870	-0.366260

Table S21. Coordinates of (**SA**)$_3$. Units are in angstrom.

Atom	X	Y	Z
S	0.167928	1.320047	-0.057411
O	-0.089819	0.122820	-0.837876
O	1.368642	2.008926	-0.384231
H	3.071998	1.295407	-0.300452
O	0.134871	0.940161	1.435600
O	-1.003405	2.277495	-0.162647
O	3.782073	0.624127	-0.246006
S	3.189524	-0.772195	0.086627
O	4.262275	-1.665797	0.230740
O	2.405779	-1.159178	-1.203415
O	-2.385102	-1.251087	-1.033280
H	1.501630	-0.787033	-1.195056
H	-1.502694	-0.804783	-1.022412
O	2.229810	-0.619051	1.147865
O	-3.143590	0.853129	-0.090075
H	0.887414	0.312052	1.592668
H	-1.882569	1.788019	-0.119931
O	-4.637305	-1.102719	-0.248887
S	-3.352713	-0.563822	-0.047144

O	-2.803894	-0.987960	1.360057
H	-3.114271	-1.875069	1.589251

Table S22. Coordinates of (**ASP**)$_3$. Units are in angstrom.

Atom	X	Y	Z
C	-4.693582	-1.007969	-0.040092
H	-4.819815	-0.671438	-1.068089
N	-4.779980	0.122093	0.852811
H	-4.864149	-0.184005	1.814473
H	-3.987520	0.746983	0.767826
C	-5.818200	-1.966929	0.284725
O	-6.341217	-2.071546	1.355302
O	-6.129003	-2.750816	-0.761291
H	-6.811042	-3.368293	-0.466779
C	-3.387219	-1.825681	0.040311
H	-3.415652	-2.645586	-0.681796
H	-3.255121	-2.245857	1.035731
O	-1.126947	-1.118384	0.333922
C	-2.170498	-0.996448	-0.280593
O	-2.343073	-0.160030	-1.269830
H	-1.492166	0.395508	-1.435056
C	-0.452500	2.100765	-0.112358
H	-0.420896	1.326536	0.653147
N	-0.292541	1.463545	-1.421030
H	-0.337914	2.162002	-2.156432
H	0.617154	1.011577	-1.497241
C	-1.837894	2.708449	-0.026878
O	-2.594035	2.562446	0.888760
O	-2.119822	3.459205	-1.101109
H	-3.014522	3.808987	-0.994318
C	0.603022	3.178055	0.218950
H	0.360029	3.652661	1.166965
H	0.633580	3.916387	-0.580020
O	2.527658	2.109667	-0.684799
C	1.930076	2.465007	0.305917
O	2.300166	2.182259	1.533769
H	3.012672	1.464902	1.493666
C	3.744611	-0.541813	-0.008000
H	4.168723	0.162050	-0.720541
N	3.912632	0.021892	1.331222
H	3.510601	-0.596433	2.028717

H	4.905100	0.117687	1.518635
C	2.277527	-0.678955	-0.385007
O	1.918680	-0.876850	-1.515471
O	1.460630	-0.605999	0.654360
H	0.526727	-0.798100	0.389567
C	4.397849	-1.911094	-0.206801
H	4.184520	-2.289752	-1.207118
H	4.000704	-2.645767	0.498131
O	6.523124	-0.882947	0.272590
C	5.891423	-1.857486	-0.030496
O	6.461016	-3.049501	-0.248826
H	7.413114	-2.948193	-0.117559

Table S23. Coordinates of (**SA**)$_2$·(**A**). Units are in angstrom.

Atom	X	Y	Z
S	-1.774334	-0.337775	-0.049575
O	-1.086230	0.169982	1.141194
O	-0.999187	-1.346365	-0.739670
O	-3.085106	-1.059623	0.450183
H	-2.865493	-1.941872	0.774429
O	-2.276400	0.741254	-0.869567
H	-1.394388	2.095824	-0.454106
O	1.436217	1.071538	-0.546266
S	2.062425	-0.121230	-0.018125
O	1.430569	-0.411659	1.363378
O	3.464214	-0.147069	0.107646
O	1.631953	-1.314038	-0.896762
H	0.441628	-0.235114	1.346365
H	0.638556	-1.367778	-0.946658
N	-0.632029	2.673580	-0.016382
H	0.250976	2.122565	-0.163002
H	-0.821004	2.7223060	0.981609
H	-0.563769	3.600938	-0.421869

Table S24. Coordinates of (**ASP**)$_2$·(**A**). Units are in angstrom.

Atom	X	Y	Z
C	2.994303	-0.108468	-0.064946
H	2.612481	0.147472	0.927622
N	2.622968	0.915382	-1.022990
H	3.306872	0.938870	-1.771618
H	1.713505	0.704301	-1.425032
C	4.503263	-0.171291	0.025989
O	5.254939	0.226598	-0.816738
O	4.916080	-0.768206	1.152887

H	5.880315	-0.816311	1.120641
C	2.483536	-1.532575	-0.404609
H	2.868739	-2.249466	0.315707
H	2.800987	-1.790794	-1.413540
O	0.315010	-0.992208	-1.231544
C	0.976698	-1.490802	-0.347404
O	0.479667	-1.961950	0.771898
H	-0.500185	-1.701912	0.834599
C	-2.266009	-0.033792	-0.021842
H	-2.158261	-0.501730	-0.998729
N	-2.046666	-1.064259	0.991369
H	-2.063604	-0.656751	1.920461
H	-2.787294	-1.753808	0.922737
C	-1.198199	1.052766	0.033202
O	-1.155273	1.927298	-0.796588
O	-0.397386	0.967681	1.074784
H	0.264977	1.751399	1.045562
C	-3.630344	0.651447	0.055309
H	-3.693499	1.442507	-0.692185
H	-3.779796	1.128219	1.027624
O	-4.665409	-1.491038	-0.329973
C	-4.768328	-0.305981	-0.167894
O	-5.954192	0.318932	-0.161102
H	-6.636941	-0.348752	-0.308951
N	1.265552	2.981655	0.727251
H	1.733276	3.562604	1.410613
H	0.668718	3.568649	0.154010
H	1.959726	2.561381	0.105256

Table S25. Coordinates of **(SA)·(A)·(ASP)**. Units are in angstrom.

Atom	X	Y	Z
S	-1.830669	-1.084095	0.144751
O	-1.415747	-0.500539	-1.143646
O	-0.705572	-1.609397	0.877472
O	-2.727329	-0.212671	0.856739
H	-0.251144	1.497551	1.785571
O	-2.735405	-2.342390	-0.225271
H	-2.159194	-3.090307	-0.419932
C	1.526556	1.005676	0.481525
H	2.356509	1.705445	0.601914
N	1.249963	0.404724	1.777952
H	0.764835	-0.482912	1.664381
H	2.108885	0.250266	2.287247
C	0.336846	1.868678	0.072270

O	0.217401	2.391915	-1.009396
O	-0.572283	2.029338	1.018083
H	-2.816545	1.753952	-0.104241
C	1.880162	0.029050	-0.633216
H	1.929111	0.540050	-1.595491
H	1.116650	-0.744858	-0.725890
O	3.952205	-0.330662	0.536397
C	3.211999	-0.613606	-0.365497
O	3.505348	-1.559278	-1.269009
H	4.370403	-1.921734	-1.038198
N	-2.517746	1.840346	-1.079073
H	-3.292183	2.089575	-1.682632
H	-2.110731	0.863462	-1.294045
H	-1.733751	2.500209	-1.148310

Table S26. Coordinates of **$(SA)_2$·(ASP)**. Units are in angstrom.

Atom	X	Y	Z
S	-1.056346	1.971581	-0.074630
O	-0.520796	3.203354	-0.591043
O	-0.313964	0.803772	-0.582226
O	-0.782192	1.986785	1.491241
H	0.039456	2.480557	1.639372
O	-2.480191	1.774058	-0.175609
H	-3.113226	0.294318	0.126561
S	-2.321298	-1.682370	-0.060067
O	-2.917218	-2.943202	-0.255849
O	-3.432146	-0.651693	0.210713
O	-1.312588	-1.561491	0.972371
H	0.193742	-1.009166	1.035993
O	-1.679747	-1.212931	-1.390493
H	-1.155979	-0.372261	-1.215102
C	1.988712	-0.784531	-0.065782
H	1.303078	-0.789274	-0.907387
N	1.190635	-0.682075	1.184204
H	1.622848	-1.267400	1.904648
H	1.142210	0.294010	1.499652
C	2.745042	-2.099554	-0.007343
O	2.866819	-2.742286	0.994935
O	3.273146	-2.408857	-1.183117
H	3.755693	-3.243318	-1.100226
C	2.997579	0.372725	-0.221028
H	3.463810	0.287469	-1.197909
H	3.754128	0.304732	0.560388
O	1.919568	2.065099	1.033202

C	2.277769	1.693317	-0.065220
O	2.047092	2.326846	-1.183635
H	1.305231	2.960116	-1.047950

Table S27. Coordinates of (**SA**)·(**ASP**)$_2$. Units are in angstrom.

Atom	X	Y	Z
S	0.138469	-1.559220	-0.212198
O	-0.138982	-0.282597	0.403737
O	0.618788	-1.505314	-1.555312
O	1.099583	-2.348397	0.687639
H	1.778600	-1.669419	1.100359
O	-1.112815	-2.450764	-0.126720
H	-1.875196	-1.916784	-0.585601
C	-3.331469	-0.060967	0.068456
H	-2.712721	-0.313044	0.933005
N	-2.820940	-0.750484	-1.113553
H	-3.594103	-1.012202	-1.718300
H	-2.183325	-0.149785	-1.632160
C	-4.741185	-0.546190	0.337395
O	-5.413498	-1.141358	-0.454098
O	-5.160543	-0.202756	1.557931
H	-6.067444	-0.519478	1.662182
C	-3.356438	1.478177	-0.064548
H	-3.824353	1.910250	0.815648
H	-3.898402	1.757581	-0.966215
O	-1.334088	1.933512	-1.233305
C	-1.930102	1.947710	-0.169424
O	-1.409643	2.295032	0.971855
H	-0.416987	2.391319	0.895885
C	3.267483	-0.002493	0.169896
H	2.743462	-0.472110	-0.668201
N	2.658984	-0.418335	1.433963
H	3.378459	-0.506465	2.145598
H	1.958891	0.253778	1.738753
C	4.703266	-0.486034	0.149633
O	5.294896	-0.884666	1.111172
O	5.243718	-0.384804	-1.066207
H	6.157275	-0.695169	-1.013982
C	3.253593	1.523334	-0.062543
H	3.762478	1.743517	-0.997697
H	3.736185	2.032645	0.768992
O	1.210586	2.366702	0.826777
C	1.815970	1.961225	-0.150968

O	1.299689	1.793884	-1.333682
H	0.307136	1.898262	-1.311629

Table S28. Coordinates of (**SA**)$_3$·(**A**). Units are in angstrom.

Atom	X	Y	Z
N	-0.074138	0.403959	2.518114
H	-0.957403	0.204028	2.002467
H	0.627612	-0.283408	2.201850
H	-0.221694	0.339982	3.519817
S	1.157167	1.966761	-0.155341
O	0.069159	1.006725	-0.314460
O	1.287722	2.458545	1.184816
H	0.294059	1.330198	2.247465
O	2.384722	1.439379	-0.754793
S	-2.906526	-0.299651	-0.114058
O	-2.216603	-1.345407	-1.026709
O	-2.501825	1.061290	-0.729947
O	-4.299762	-0.439901	-0.256763
O	-2.315441	-0.400593	1.197068
H	-1.292210	-1.541146	-0.750737
H	-1.523294	1.195184	-0.622965
S	1.614715	-1.753279	-0.067360
O	2.473079	-3.062793	-0.056358
O	2.231827	-0.970417	-1.201227
O	0.270285	-2.139600	-0.372956
O	1.863285	-1.122153	1.190528
H	2.148688	-3.682610	-0.723169
H	2.319860	0.075481	-1.010756
O	0.794201	3.244587	-1.004282
H	0.952443	3.075978	-1.941954

Table S29. Coordinates of (**ASP**)$_3$(**A**). Units are in angstrom.

Atom	X	Y	Z
C	-0.722585	2.106524	0.776877
H	-1.359293	1.281710	1.095414
N	0.016430	2.592602	1.940261
H	0.727526	3.253357	1.644293
H	-0.606108	3.060103	2.587185
C	0.291820	1.543293	-0.210410
O	1.478241	1.768981	-0.083887
O	-0.250295	0.832108	-1.156182
H	0.490472	0.347589	-1.703566
C	-1.599261	3.158184	0.070679
H	-1.009044	3.814942	-0.564766
H	-2.086439	3.762063	0.838745
O	-2.947842	2.811170	-1.898023
C	-2.708455	2.545505	-0.757906
O	-3.423546	1.691274	-0.017195
H	-4.149323	1.278632	-0.524466
C	-3.725443	-1.366818	0.648149
H	-3.474608	-0.421368	1.124679
N	-3.797578	-2.391371	1.672227
H	-4.027650	-3.292750	1.271073
H	-2.893144	-2.466037	2.121514
C	-5.059405	-1.159234	-0.033255
O	-5.378699	-0.147061	-0.606014
O	-5.841291	-2.237733	-0.016523
H	-6.643766	-2.028556	-0.513149
C	-2.701471	-1.617543	-0.465127
H	-2.739667	-0.824708	-1.218065
H	-2.895314	-2.561311	-0.976398
O	-0.444720	-2.150332	-0.781607
C	-1.280114	-1.620165	0.044002
O	-0.976007	-1.127245	1.126318
H	0.682277	-0.578159	1.657501
C	4.456486	-0.624244	0.151870
H	4.224652	-1.608732	0.566868
N	3.893042	0.413008	1.014487
H	4.628405	0.782282	1.609825
H	3.554675	1.187109	0.448590

C	5.969806	-0.527173	0.109952
O	6.622584	0.279483	0.710922
O	6.516625	-1.479263	-0.656966
H	7.475623	-1.370405	-0.619720
C	3.861825	-0.565813	-1.250004
H	4.307151	-1.339068	-1.875481
H	4.064020	0.396930	-1.719786
O	1.708219	-0.324378	-2.204917
C	2.354065	-0.784802	-1.248277
O	1.868738	-1.424064	-0.271928
H	0.545728	-1.884568	-0.540506
N	1.347563	-0.014817	2.220410
H	1.442834	-0.439570	3.136996
H	0.955247	0.946100	2.310010
H	2.289867	0.038668	1.740230

Table S30. Coordinates of (**SA**)$_2$·(**A**)·(**ASP**). Units are in angstrom.

Atom	X	Y	Z
S	1.400981	-1.920777	-0.413130
O	0.834938	-3.213235	-0.733527
O	0.490264	-0.821033	-0.735821
O	1.585222	-1.883649	1.165991
H	0.730821	-2.131524	1.566378
O	2.746642	-1.696202	-0.889189
H	3.507767	-0.503522	0.033962
S	1.381214	2.349897	-0.063853
O	2.239676	3.482965	-0.049875
O	1.462983	1.493610	1.135016
O	-0.027917	2.608691	-0.372765
H	-0.852959	1.604941	0.382182
O	1.937778	1.441198	-1.237044
H	1.414525	0.609295	-1.262736
C	-2.380377	0.233945	-0.088628
H	-1.903696	0.096794	-1.057996
N	-1.359941	0.757619	0.839064
H	-1.782114	1.054438	1.718046
H	-0.624918	0.065212	1.012807
C	-3.479575	1.274941	-0.172107
O	-3.663303	2.099695	0.674170
O	-4.230009	1.113832	-1.257130
H	-4.930876	1.780149	-1.246961
C	-2.991795	-1.092742	0.397598
H	-3.739465	-1.414746	-0.321859
H	-3.444472	-0.950596	1.377987

O	-1.139463	-2.110479	1.470128
C	-1.872807	-2.100402	0.500908
O	-1.740595	-2.843934	-0.560086
H	-0.808382	-3.205403	-0.608322
N	3.766479	0.275499	0.685738
H	4.318134	-0.077062	1.460453
H	2.853851	0.716833	1.023730
H	4.278478	0.991319	0.174894

Table S31. Coordinates of (**SA**)·(**A**)·(**ASP**)$_2$. Units are in angstrom.

Atom	X	Y	Z
S	0.466486	-1.664025	-1.347326
O	0.840584	-2.966455	-0.811135
O	0.255332	-0.691260	-0.280257
O	1.659141	-1.155985	-2.210786
H	2.415163	-0.934445	-1.573957
O	-0.662420	-1.714451	-2.267778
H	-1.900332	-0.993486	-1.608057
C	2.912579	0.980177	-0.024044
H	1.987502	1.193397	-0.563502
N	3.285503	-0.413672	-0.230445
H	4.296470	-0.503432	-0.215112
H	2.889770	-0.991909	0.505700
C	4.006116	1.861409	-0.587517
O	5.120575	1.494185	-0.826317
O	3.595143	3.123475	-0.756837
H	4.344987	3.633637	-1.089525
C	2.698850	1.365542	1.458078
H	2.505085	2.432264	1.531702
H	3.584502	1.096446	2.031431
O	1.631243	-0.556865	2.370226
C	1.512159	0.590562	1.976735
O	0.391949	1.247276	1.906815
H	-0.411533	0.635084	2.065621
C	-2.503627	0.194887	0.055925
H	-1.642247	0.822353	-0.155336
N	-2.795046	-0.610452	-1.158866
H	-3.314923	-1.438499	-0.854140
H	-3.311246	-0.052014	-1.840530
C	-2.145924	-0.786219	1.188915
O	-1.577974	-0.307273	2.190945
O	-2.490826	-1.967251	1.015935
H	-0.987995	-2.675511	1.696664
C	-3.706672	1.023512	0.489532

H	-3.450509	1.570270	1.394217
H	-4.548347	0.371943	0.744774
O	-4.041736	1.834511	-1.750639
C	-4.193365	1.982052	-0.564924
O	-4.854562	3.016617	-0.048765
H	-5.169134	3.566264	-0.779719
N	0.039050	-2.801548	1.778244
H	0.267811	-3.542752	2.430118
H	0.455308	-1.905193	2.090180
H	0.407051	-3.004042	0.816692

Table S32. Coordinates of (**SA**)$_2$·(**A**)$_2$. Units are in angstrom.

Atom	X	Y	Z
S	-2.046022	0.037836	-0.132939
O	-1.998061	1.453980	0.193118
O	-3.442196	-0.186985	-0.850278
O	-1.092613	-0.386094	-1.132718
O	-2.044028	-0.811632	1.046246
H	-0.592046	2.195674	0.681064
H	-4.150366	0.123114	-0.273117
S	2.129139	-0.075273	-0.203764
O	1.997404	-1.453253	-0.660918
O	1.294574	0.817481	-1.215729
O	1.414222	0.073599	1.088308
O	3.435399	0.485438	-0.212892
H	0.817552	-2.109878	0.179257
H	0.410300	0.400324	-1.347298
N	0.148807	-2.437668	0.943566
H	-0.095772	-3.415310	0.829993
H	0.636376	-2.290591	1.823564
H	-0.711759	-1.840511	0.949632
N	0.382209	2.455188	0.968733
H	0.383658	3.082179	1.764838
H	0.872385	1.517336	1.174992
H	0.865075	2.873727	0.177110

Table S33. Coordinates of (**ASP**)$_2$·(**A**)$_2$. Units are in angstrom.

Atom	X	Y	Z
C	2.467264	-0.062632	0.171125
H	1.813175	0.588140	0.755602
N	3.308276	-0.815319	1.084784
H	3.781120	-1.564800	0.592951
H	3.988093	-0.202436	1.516040
C	1.561933	-1.023068	-0.592675

O	0.720415	-0.403043	-1.384122
O	1.649631	-2.224056	-0.481553
H	-0.684019	-2.961957	-1.789211
C	3.223410	0.803321	-0.841220
H	2.530889	1.298368	-1.522315
H	3.886582	0.192525	-1.458486
O	4.124079	2.061746	1.007657
C	4.054842	1.863678	-0.173913
O	4.738716	2.597317	-1.066032
H	5.243984	3.256275	-0.572330
C	-2.467263	-0.062632	-0.171125
H	-1.813174	0.588140	-0.755602
N	-3.308276	-0.815319	-1.084783
H	-3.781120	-1.564800	-0.592950
H	-3.988093	-0.202437	-1.516040
C	-1.561933	-1.023067	0.592675
O	-0.720414	-0.403042	1.384122
O	-1.649630	-2.224056	0.481554
H	0.684019	-2.961956	1.789212
C	-3.223409	0.803322	0.841220
H	-2.530888	1.298370	1.522313
H	-3.886581	0.192526	1.458487
O	-4.124081	2.061744	-1.007658
C	-4.054842	1.863678	0.173913
O	-4.738717	2.597317	1.066031
H	-5.243986	3.256273	0.572328
N	0.890987	-2.172011	2.391682
H	0.838116	-2.472612	3.356118
H	-0.106499	-1.098045	1.861840
H	1.842543	-1.867651	2.176190
N	-0.890987	-2.172012	-2.391681
H	0.106499	-1.098047	-1.861839
H	-1.842543	-1.867653	-2.176190
H	-0.838116	-2.472614	-3.356117

Table S34. Coordinates of (**SA**)·(**A**)$_2$·(**ASP**). Units are in angstrom.

Atom	X	Y	Z
S	-1.804066	-1.076729	-0.389109
O	-3.209279	-0.849213	-0.567305
O	-1.396720	-2.481097	-0.432317
O	-1.056459	-0.476783	-1.664057
H	-1.038936	0.494351	-1.585200
O	-1.228307	-0.394799	0.763064
H	-0.285609	-2.587439	2.355339

C	1.731670	0.206119	0.039290
H	1.007568	-0.356976	-0.552800
N	1.582461	-0.143421	1.448120
H	2.456913	0.034231	1.932394
H	0.856212	0.441262	1.856071
C	3.111645	-0.213842	-0.416173
O	3.984526	-0.594477	0.312309
O	3.258187	-0.098094	-1.739702
H	4.157998	-0.368495	-1.963933
C	1.534666	1.708360	-0.271198
H	1.639283	1.871446	-1.340531
H	2.282357	2.286505	0.270953
O	-0.052273	2.406035	1.362314
C	0.164433	2.146641	0.202482
O	-0.750453	2.175241	-0.747127
H	-1.704851	2.230480	-0.298187
N	-3.019182	1.994496	0.455241
H	-2.651543	1.811600	1.383798
H	-3.451045	1.129789	0.131479
H	-3.719964	2.721400	0.517258
N	0.320159	-2.609279	1.539802
H	0.875565	-1.687263	1.522824
H	-0.326321	-2.649871	0.678891
H	0.935128	-3.414101	1.591418

Table S35. Coordinates of $(\mathbf{SA})_3 \cdot (\mathbf{A})_2$. Units are in angstrom.

Atom	X	Y	Z
N	-0.000759	-2.032414	0.157616
H	-0.793117	-2.156394	-0.492713
H	0.918403	-1.943622	-0.317617
H	0.010093	-2.791360	0.831929
N	-2.354751	1.899760	1.656060
H	-3.292294	2.180192	1.380256
H	-2.128090	2.261507	2.576750
H	-2.321300	0.857073	1.643426
S	-3.068695	-0.820949	-0.131153
O	-2.542076	-1.873978	-0.968841
O	-2.976352	0.500950	-0.737607
O	-2.549699	-0.826749	1.227763
H	-1.356863	0.631814	-1.386962
S	0.290679	1.514282	-0.396409
O	-0.373826	0.604941	-1.485441
O	1.588157	1.846796	-0.914086
O	-0.598745	2.642793	-0.186460

O	0.359271	0.687931	0.827614
H	-0.154188	-1.135816	0.642368
H	-1.663657	2.259630	0.929587
O	-4.612441	-1.118389	0.067998
H	-5.015769	-1.300875	-0.790194
S	3.465521	-0.696953	0.133606
O	3.889900	0.620830	-0.547337
O	2.746174	-0.241905	1.436137
O	4.627491	-1.401467	0.504448
O	2.484717	-1.340769	-0.704392
H	3.081404	1.137344	-0.805758
H	1.863307	0.179150	1.238126

Table S36. Coordinates of (**ASP**)$_3$·(**A**)$_2$. Units are in angstrom.

Atom	X	Y	Z
C	-0.618865	1.863752	-0.123609
H	-0.424603	0.855125	0.231354
N	-0.810562	1.787215	-1.599241
H	-1.496668	2.509863	-1.842967
H	0.097672	1.911914	-2.061791
C	-1.916655	2.415869	0.499556
O	-2.183421	2.041549	1.663338
O	-2.574014	3.199509	-0.204534
H	-4.230176	2.541093	0.458028
C	0.534031	2.795769	0.241854
H	0.619068	2.843065	1.324083
H	0.315135	3.805119	-0.117354
O	2.875587	2.504600	0.433140
C	1.856316	2.369145	-0.363754
O	1.931378	1.952641	-1.508020
H	5.245137	2.341490	-1.573659
C	-3.275857	-2.130433	-0.719439
H	-4.357376	-2.005093	-0.705261
N	-2.923918	-3.216119	-1.611775
H	-1.912867	-3.264662	-1.695049
H	-3.234158	-4.100113	-1.226581
C	-2.696074	-0.815265	-1.241447
O	-3.331356	0.239868	-1.057437
O	-1.569135	-0.837167	-1.809872
H	-1.195778	0.837600	-1.841046
C	-2.800659	-2.365215	0.745765
H	-1.765025	-2.698464	0.724523
H	-3.431170	-3.135860	1.184593
O	-3.985388	-0.651111	1.931506

C	-2.926035	-1.094696	1.539922
O	-1.774050	-0.470110	1.679377
H	-1.925275	0.509213	1.883256
C	3.226101	-1.028801	0.153455
H	2.643640	-0.142986	0.413489
N	3.611165	-0.913456	-1.239434
H	4.107363	-1.739217	-1.553217
H	2.783356	-0.782054	-1.807575
C	4.469061	-0.976571	1.021051
O	5.597576	-0.934135	0.620585
O	4.161492	-0.981296	2.326389
H	4.988929	-0.938936	2.822511
C	2.388202	-2.264877	0.507715
H	2.165539	-2.279956	1.575348
H	2.927418	-3.184081	0.277651
O	0.397602	-3.323750	-0.294597
C	1.056552	-2.319484	-0.213236
O	0.690055	-1.152372	-0.713609
H	-0.221639	-1.208516	-1.137787
N	5.020922	1.718041	-0.807555
H	4.707117	0.823944	-1.199102
H	3.763651	2.221871	-0.048706
H	5.871165	1.532523	-0.288442
N	-4.761788	1.667294	0.607848
H	-4.525393	1.275537	1.524915
H	-4.371871	0.974389	-0.092670
H	-5.761223	1.795385	0.505418

Table S37. Coordinates of (**SA**)$_2$·(**A**)$_2$·(**ASP**). Units are in angstrom.

Atom	X	Y	Z
S	-2.977224	-1.234550	-0.364414
O	-4.095697	-1.823708	-1.011959
O	-2.265280	-0.349963	-1.467229
O	-3.346235	-0.262402	0.698215
H	-3.658614	1.183866	-0.029398
O	-1.960164	-2.140199	0.155955
H	-0.453128	-2.222377	-0.368836
S	-0.165911	1.999558	0.274837
O	-1.106802	2.817323	-0.484001
O	-0.298642	2.167251	1.706711
O	-0.255393	0.578710	-0.109881
H	-1.442962	0.043296	-1.059608

O	1.252442	2.458611	-0.123926
H	1.728729	1.728904	-0.682380
C	3.041148	-0.252433	-0.177836
H	2.742659	0.210925	0.766631
N	2.366006	0.412988	-1.288828
H	2.996876	0.479056	-2.081896
H	1.528367	-0.093540	-1.559834
C	4.535387	-0.051827	-0.334055
O	5.066344	0.323832	-1.338898
O	5.198937	-0.371684	0.780158
H	6.141679	-0.242054	0.612601
C	2.746610	-1.761316	-0.073576
H	3.367579	-2.190764	0.708751
H	2.947317	-2.245265	-1.027550
O	0.504197	-2.204805	-0.672802
C	1.301862	-1.942697	0.329091
O	0.950068	-1.807233	1.481943
H	-1.365866	-0.600418	3.435102
N	-1.191575	-0.352342	2.467741
H	-0.510364	-1.010492	2.043203
H	-0.805779	0.608044	2.383223
H	-2.067963	-0.386281	1.911395
N	-3.612876	2.028247	-0.661960
H	-3.775766	1.696706	-1.609838
H	-2.617062	2.409590	-0.595884
H	-4.296646	2.732180	-0.407152

Table S38. Coordinates of (**SA**)·(**A**)$_2$·(**ASP**)$_2$. Units are in angstrom.

Atom	X	Y	Z
S	-3.509378	0.479305	-0.136532
O	-2.871898	1.787437	-0.090039
O	-4.855221	0.439212	-0.610660
O	-2.690976	-0.394601	-1.159623
H	-4.236517	-2.241799	-0.867583
O	-3.331806	-0.208893	1.165566
H	-1.868575	0.412453	1.795910
C	2.055481	-2.148711	-0.020529
H	1.938396	-1.465708	0.820259
N	2.110825	-1.355887	-1.245320
H	2.526483	-1.900918	-1.994205
H	1.166862	-1.081419	-1.498581
C	3.371252	-2.876592	0.129173
O	4.148163	-3.071340	-0.761153
O	3.554965	-3.328252	1.377023

H	4.391544	-3.811168	1.393542
C	0.924688	-3.180931	0.008546
H	0.959170	-3.758188	0.932879
H	1.031294	-3.893328	-0.811806
O	-1.419314	-3.362579	-0.179754
C	-0.465042	-2.561439	-0.095630
O	-0.553694	-1.306732	-0.097747
H	-1.830962	-0.728589	-0.736445
C	2.561815	3.067320	0.298608
H	2.350291	3.307063	1.338617
N	3.902863	3.495110	-0.040246
H	4.163019	3.154796	-0.958086
H	3.969430	4.504762	-0.043984
C	2.431117	1.560987	0.163131
O	1.701917	0.914165	0.889484
O	3.095209	1.058853	-0.843374
H	2.807671	0.083101	-0.996098
C	1.447089	3.699499	-0.573408
H	1.612808	3.463400	-1.622235
H	1.486059	4.779673	-0.434860
O	-0.316632	3.397057	1.002709
C	0.087474	3.220180	-0.129366
O	-0.571873	2.559575	-1.050573
H	-1.473063	2.276130	-0.718815
N	-3.891842	-2.653651	-0.001357
H	-3.899994	-1.891391	0.699036
H	-2.833662	-2.948167	-0.123908
H	-4.476403	-3.431268	0.282805
N	-0.907960	0.813931	1.889196
H	-0.284472	0.326182	1.233783
H	-0.530619	0.706521	2.824883
H	-0.909881	1.819359	1.635478