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Supplementary Information: Does phosphorylation increase the binding affinity of aluminum? A computational study on the Aluminum interaction with serine and O-phosphoserine

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Abbreviations used to indicate the different coordination modes: mC, monodentate binding of carboxylate; bC, bidentate binding of carboxylate; O, monodentate binding of alkoxide group; mP, monodentate binding of phosphate group; bP, bidentate binding of phosphate group; N monodentate binding of amine group; dCO dicoordinate binding of carboxylate and alkoxide groups; ; dCP dicoordinate binding of carboxylate and phosphate groups; dCN dicoordinate binding of carboxylate and amine groups; $tCNO$ tricoordinate binding of carboxylate, amine and alkoxide groups; $tCNP$ tricoordinate binding of carboxylate, amine and phosphate groups; tCP tricoordinate binding of carboxylate monodentately and phosphate bidentately; $tCNbP$ tetracoordinate binding of carboxylate and amine groups monodentately and phosphate group bidentately.

Figure S1: Complexation enthalpies and free energies for Al-Ser (filled symbols) and Al-PSer (striped symbols) complexes: A) Al^{3+} complexes; B) $[Al(OH)]^{2+}$ complexes; and C) $[Al(OH)_2]^{1+}$ complexes. The symbols denote the different protonation state of the titrable groups, which are written in parentheses: NH_3^+ and OH (spheres), NH_3^+ and O^- (squares), NH_2 and OH (stars), NH_2 and O^- (diamonds), NH_3^+ and $OHPO_3^-$ (triangles up), NH_3^+ and OPO_3^{-2} (triangles down) and NH_2 and OPO_3^{-2} (triangles left). The different colors account for the different binding modes of the complexes: monodentate binding of carboxylate group (black), bidentate binding of carboxylate group (red), amine group (yellow), binding of alkoxide or monodentate phosphate group (blue), bidentate binding of phosphate group (brown), dicoordinate binding of carboxylate and alkoxide or monodentate phosphate groups (orange), dicoordinate binding of carboxylate and amine groups (cyan), tricoordinate binding of carboxylate and bidentate phosphate groups (green), tricoordinate binding of carboxylate, amine and monodentate phosphate groups (magenta) and tetracoordinate binding of carboxylate, amine and bidentate phosphate groups (violet). R stands for alkoxide or monodentate phosphate.

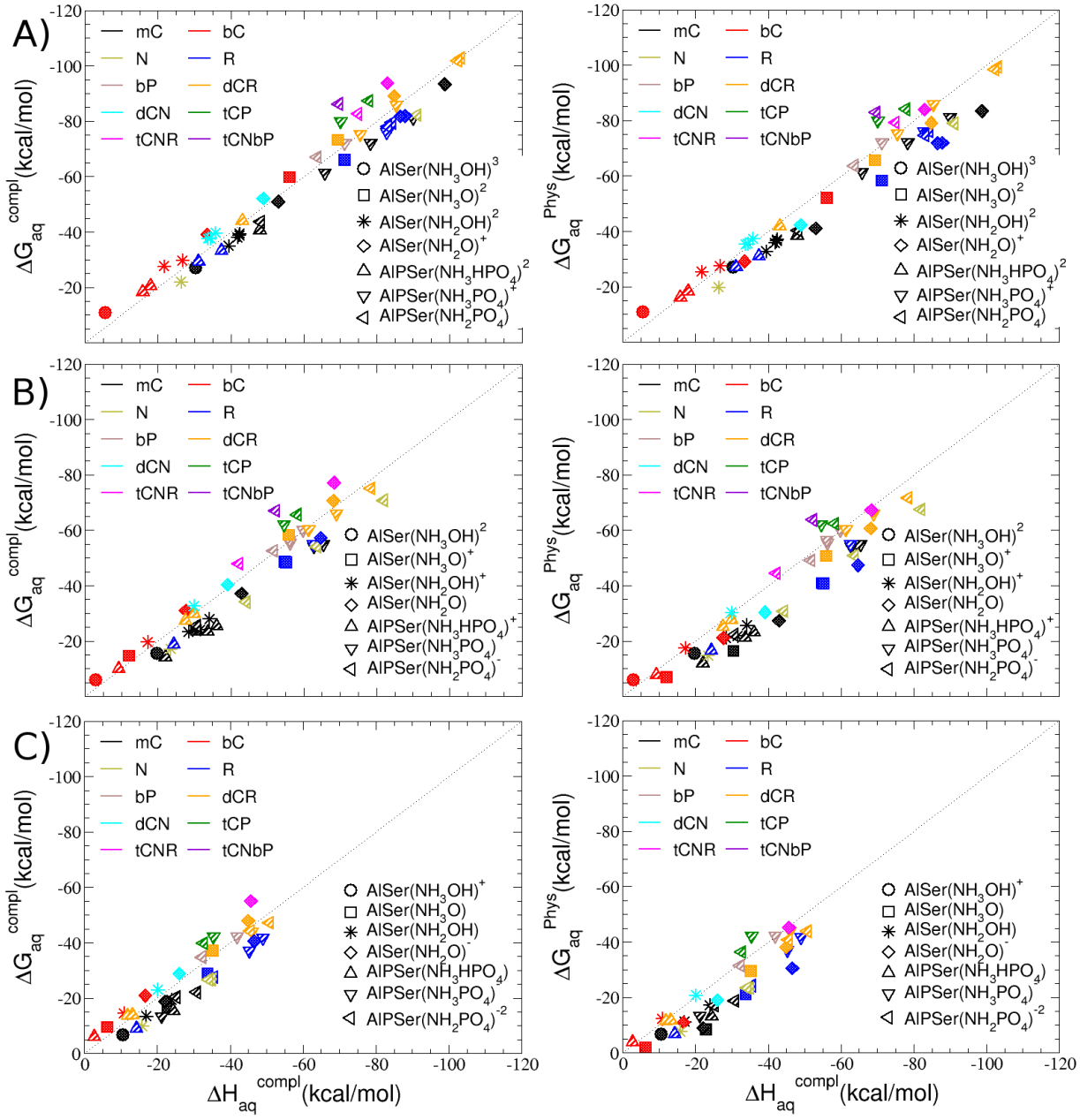


Table S1: Complexation free energy affinities in kcal/mol for representative complexes with different functionals: B3LYP-D3BJ, PBE0-D3BJ, TPSS-D3BJ, B97D3 and M062X. The † sign indicates a spontaneous proton transfer from a water molecule to alkoxide/phosphate group during the optimization.

	Structure	B3LYP-D3BJ	PBE0-D3BJ	TPSS-D3BJ	B97D3	M062X
Al^{3+}	$[Al(Ser)_O(H_2O)_5]^2$	-65.91	-67.69	-67.83	-65.52	-66.81
	$[Al(Ser)_{dCO}(H_2O)_4]^2$	-73.21	-73.64	-72.89	-72.00	-73.48
	$[Al(Ser)_O(H_2O)_5]^1$	-81.80	-82.60	-82.74	-80.88	-82.58
	$[Al(Ser)_{dCO}(H_2O)_4]^1$	-88.95	-89.45	-88.87	-88.33	-89.13
	$[Al(Ser)_{mC}(H_2O)_5]^1$ (†)	-93.31	-94.37	-94.14	-92.12	-93.83
	$[Al(Ser)_{tCNO}(H_2O)_3]^1$	-93.73	-95.58	-97.02	-95.42	-91.69
	$[Al(PSer)_{mC}(H_2O)_5]^1$ (†)	-81.14	-81.00	-82.75	-80.62	-79.13
	$[Al(PSer)_{tCNP}(H_2O)_3]$	-82.53	-83.75	-87.41	-86.24	-78.49
	$[Al(PSer)_{dCP}(H_2O)_4]^1$	-85.66	-85.96	-86.45	-85.03	-85.56
	$[Al(PSer)_{tCNbP}(H_2O)_2]$	-86.20	-88.30	-91.72	-90.10	-83.05
	$[Al(PSer)_{tCP}(H_2O)_3]$	-87.36	-88.31	-89.22	-88.83	-86.13
	$[Al(PSer)_{dCP}(H_2O)_4]$ (†)	-102.74	-103.62	-104.28	-102.41	-102.08
$[Al(OH)]^{2+}$	$[Al(Ser)_{dCN}(H_2O)_3(OH)]$	-40.20	-40.22	-42.33	-43.23	-35.98
	$[Al(Ser)_O(H_2O)_4(OH)]^1$	-48.54	-49.14	-48.95	-47.52	-49.05
	$[Al(Ser)_O(H_2O)_4(OH)]$	-57.16	-57.72	-57.76	-56.49	-58.34
	$[Al(Ser)_{dCO}(H_2O)_3(OH)]^1$	-58.27	-58.60	-57.95	-57.20	-58.57
	$[Al(Ser)_{dCO}(H_2O)_3(OH)]$	-70.53	-70.96	-70.45	-70.14	-70.74
	$[Al(Ser)_{tCNO}(H_2O)_2(OH)]$	-77.13	-78.63	-79.90	-78.52	-75.31
	$[Al(PSer)_{bP}(H_2O)_3(OH)]$	-59.97	-60.87	-62.27	-61.26	-57.83
	$[Al(PSer)_{tCP}(H_2O)_2(OH)]$	-62.06	-62.50	-63.52	-63.29	-60.63
	$[Al(PSer)_{tCP}(H_2O)_2(OH)]^-$	-65.61	-66.29	-67.28	-67.03	-64.43
	$[Al(PSer)_{dCP}(H_2O)_3(OH)]$	-65.98	-66.73	-67.41	-65.30	-67.07
	$[Al(PSer)_{tCNbP}(H_2O)(OH)]^-$	-67.01	-68.74	-71.89	-70.58	-64.10
	$[Al(PSer)_{dCP}(H_2O)_3(OH)]^-$	-75.04	-75.94	-77.96	-75.39	-74.54
$[Al(OH)_2]^+$	$[Al(Ser)_O(H_2O)_3(OH)_2]$	-28.68	-29.13	-29.21	-27.62	-29.47
	$[Al(Ser)_{dCN}(H_2O)_2(OH)_2]^-$	-28.79	-28.68	-30.19	-30.64	-25.60
	$[Al(Ser)_{dCO}(H_2O)_2(OH)_2]$	-37.13	-37.42	-37.51	-36.69	-36.66
	$[Al(Ser)_O(H_2O)_3(OH)_2]^-$	-40.40	-40.52	-40.49	-39.64	-40.82
	$[Al(Ser)_{dCO}(H_2O)_2(OH)_2]^-$	-47.87	-48.55	-48.85	-47.89	-47.56
	$[Al(Ser)_{tCNO}(H_2O)(OH)_2]^-$	-55.01	-55.70	-57.20	-56.86	-52.47
	$[Al(PSer)_{tCP}(H_2O)(OH)_2]^{-2}$	-39.70	-39.44	-40.84	-40.62	-37.40
	$[Al(PSer)_{mP}(H_2O)_3(OH)_2]^-$	-41.62	-41.56	-41.59	-40.31	-40.37
	$[Al(PSer)_{tCP}(H_2O)(OH)_2]^-$	-42.10	-42.48	-43.92	-42.91	-41.72
	$[Al(PSer)_{bP}(H_2O)_2(OH)_2]^-$	-42.22	-43.06	-43.42	-42.50	-41.09
	$[Al(PSer)_{dCP}(H_2O)_2(OH)_2]^-$	-43.85	-43.52	-44.76	-43.14	-42.56
	$[Al(PSer)_{dCP}(H_2O)_2(OH)_2]^{-2}$	-47.18	-46.54	-48.35	-46.50	-45.70

Al^{3+} species

Table S2: Enthalpy and free energy affinities in kcal/mol for $Al^{3+} - Ser$ complexes formation with corrections that account for the physiological pH and deprotonation of the corresponding titratable groups. The subscripts indicate the coordination mode of Ser to Al^{3+}. The † sign indicates a spontaneous proton transfer from a water molecule to alkoxide group during the optimization. The § sign indicates a spontaneous proton transfer from a water molecule to carboxilate group during the geometry optimization. The $ sign indicates two spontaneous proton transfer from a water molecule to the alkoxide group and from another water molecule to the amine group during the optimization.

$Al^{3+} - Ser$ **Complexes**

Titratable groups	Structure	ΔH_{aq}^{compl}	ΔG_{aq}^{compl}	ΔG_{aq}^{Phys}
NH_3^+, COO^-, OH	$[Al(Ser)_{mC}(H_2O)_5]^3$	-30.38	-27.01	-27.01
	$[Al(Ser)_{bC}(H_2O)_4]^3$	-5.57	-10.69	-10.69
NH_3^+, COO^-, O^-	$[Al(Ser)_{bC}(H_2O)_4]^2$ (†)	-56.18	-59.71	-52.06
	$[Al(Ser)_{O}(H_2O)_5]^2$	-71.21	-65.91	-58.27
	$[Al(Ser)_{dCO}(H_2O)_4]^2$	-69.36	-73.21	-65.57
NH_2, COO^-, OH	$[Al(Ser)_{mC}(H_2O)_5]^2$	-42.32	-38.73	-36.48
	$[Al(Ser)_{mC}(H_2O)_5]^2$	-42.47	-39.29	-37.04
	$[Al(Ser)_{mC}(H_2O)_5]^2$	-39.51	-34.90	-32.65
	$[Al(Ser)_{mC}(H_2O)_5]^2$	-41.94	-38.03	-35.78
	$[Al(Ser)_{bC}(H_2O)_4]^2$	-26.77	-29.66	-27.41
	$[Al(Ser)_{bC}(H_2O)_4]^2$	-21.75	-27.55	-25.30
	$[Al(Ser)_{N}(H_2O)_5]^2$	-26.37	-21.93	-19.68
	$[Al(Ser)_{dCN}(H_2O)_4]^2$	-33.79	-37.55	-35.30
	$[Al(Ser)_{dCN}(H_2O)_4]^2$	-35.87	-39.54	-37.29
	$[Al(Ser)_{dCN}(H_2O)_4]^2$	-34.43	-37.69	-35.44
NH_2, COO^-, O^-	$[Al(Ser)_{mC}(H_2O)_5]^1$ (†)	-98.69	-93.31	-83.41
	$[Al(Ser)_{mC}(H_2O)_5]^1$ (§)	-53.07	-50.87	-40.97
	$[Al(Ser)_{mC}(H_2O)_5]^1$ ($)	-98.89	-93.19	-83.29
	$[Al(Ser)_{bC}(H_2O)_4]^1$	-33.50	-38.97	-29.08
	$[Al(Ser)_{O}(H_2O)_5]^1$	-87.95	-81.80	-71.91
	$[Al(Ser)_{O}(H_2O)_5]^1$ (§)	-86.56	-81.67	-71.78
	$[Al(Ser)_{dCO}(H_2O)_4]^1$	-84.86	-88.95	-79.05
	$[Al(Ser)_{dCN}(H_2O)_4]^1$	-48.95	-52.07	-42.18
	$[Al(Ser)_{tCNO}(H_2O)_3]^1$	-83.06	-93.73	-83.84

Table S3: Enthalpy and free energy affinities in kcal/mol for $Al^{3+} - PSer$ complexes formation with corrections that account for the physiological pH and de/protonation of the corresponding titratable groups. The subscripts indicate the coordination mode of PSer to Al^{3+}. The † sign indicates a spontaneous proton transfer from a water molecule to the phosphate group during the optimization. The ‡ sign indicates two spontaneous proton transfer from a water molecule to the phosphate group and from another water molecule to carboxylate group during the optimization. The § sign indicates a spontaneous proton transfer from amine to phosphate group during the optimization.

$Al^{3+} - PSer$ **Complexes**

Titratable groups	Structure	ΔH_{aq}^{compl}	ΔG_{aq}^{compl}	ΔG_{aq}^{Phys}
NH_3^+, COO^-, $OHPO_3^-$	$[Al(PSer)_{mC}(H_2O)_5]^2$	-47.98	-40.65	-38.44
	$[Al(PSer)_{bC}(H_2O)_4]^2$	-17.96	-20.38	-18.17
	$[Al(PSer)_{bC}(H_2O)_4]^2$	-15.86	-18.17	-15.96
	$[Al(PSer)_{mP}(H_2O)_5]^2$	-37.51	-33.31	-31.10
	$[Al(PSer)_{mP}(H_2O)_5]^2$	-31.18	-29.27	-27.06
	$[Al(PSer)_{dCP}(H_2O)_4]^2$	-43.16	-44.10	-41.89
NH_3^+, COO^-, OPO_3^{-2}	$[Al(PSer)_{mC}(H_2O)_5]^1$ (†)	-90.05	-81.14	-81.14
	$[Al(PSer)_{mC}(H_2O)_5]^1$ (†)	-78.43	-72.05	-72.05
	$[Al(PSer)_{mC}(H_2O)_5]^1$ (§)	-65.90	-61.13	-61.13
	$[Al(PSer)_{mP}(H_2O)_5]^1$	-82.91	-75.93	-75.93
	$[Al(PSer)_{bP}(H_2O)_4]^1$	-71.33	-72.05	-72.05
	$[Al(PSer)_{dCP}(H_2O)_4]^1$	-85.44	-85.66	-85.66
	$[Al(PSer)_{dCP}(H_2O)_4]^1$	-75.55	-75.20	-75.20
	$[Al(PSer)_{tCP}(H_2O)_3]^1$	-70.22	-79.76	-79.76
NH_2, COO^-, OPO_3^{-2}	$[Al(PSer)_{mC}(H_2O)_5]$	-48.16	-43.57	-40.22
	$[Al(PSer)_{mP}(H_2O)_5]$ (†)	-84.25	-79.36	-76.02
	$[Al(PSer)_{mP}(H_2O)_5]$ (†)	-53.21	-77.98	-74.63
	$[Al(PSer)_{bP}(H_2O)_4]$	-63.77	-66.97	-63.63
	$[Al(PSer)_{N}(H_2O)_5]$ (‡)	-91.15	-82.20	-78.85
	$[Al(PSer)_{dCP}(H_2O)_4]$ (†)	-103.22	-102.74	-99.39
	$[Al(PSer)_{dCP}(H_2O)_4]$ (†)	-102.33	-101.69	-98.35
	$[Al(PSer)_{tCP}(H_2O)_3]$	-77.92	-87.36	-84.02
	$[Al(PSer)_{tCNP}(H_2O)_3]$	-75.02	-82.53	-79.18
	$[Al(PSer)_{tCNbP}(H_2O)_2]$	-69.76	-86.20	-82.85

Table S4: Distance (in Å) and electron delocalitation indexes (DI) of the first coordination sphere of aluminum and of hydrogen bonds in representative $Al^{3+} - Ser$ structures. QTAIM parameters of $Al...O$ and $Al...N$ bond critical points (BCP, in au): ρ_{BCP}, the electron density at BCP; ∇^2_{BCP}, the laplacian of the electron density; and H_{BCP}, the total electron energy density at BCP. O_C stands for carboxylate group oxygen atom, O for alkoxide oxygen atom, and O_W for water molecule. The subscripts indicate the coordination mode of Ser to Al^{3+}.

$Al^{3+} - Ser$ Complexes

Titrable groups	Structure	Distance		DI	ρ_{BCP}	∇^2_{BCP}	H_{BCP}
NH_3^+, COO^-, O^-	$[Al(Ser)_{dCO}(H_2O)_4]^2$	Al-O_C	1.844	0.180	0.0697	0.5118	0.0063
		Al-O	1.779	0.226	0.0854	0.6698	0.0053
		Al-O_{W1}	1.947	0.127	0.0511	0.3412	0.0053
		Al-O_{W2}	1.966	0.123	0.0492	0.3150	0.0042
		Al-O_{W3}	1.979	0.121	0.0471	0.3036	0.0046
		Al-O_{W4}	1.988	0.122	0.0469	0.2941	0.0038
		H_N-O_C	2.032	0.063	0.0261	0.0927	0.0013
	$[Al(Ser)_O(H_2O)_5]^2$	Al-O	1.768	0.220	0.0843	0.6847	0.0076
		Al-O_{W1}	1.924	0.151	0.0573	0.3783	0.0042
		Al-O_{W2}	1.958	0.126	0.0497	0.3274	0.0050
		Al-O_{W3}	1.937	0.142	0.0544	0.3593	0.0047
		Al-O_{W4}	1.962	0.124	0.0495	0.3180	0.0042
		Al-O_{W5}	1.951	0.129	0.0506	0.3356	0.0051
		H_{W1}-O_C	1.517	0.156	0.0712	0.1601	-0.0135
		H_{W3}-O_C	1.698	0.104	0.0441	0.1307	-0.0009
		H_N-O_C	1.905	0.086	0.0336	0.1071	0.0001
NH_2, COO^-, O^-	$[Al(Ser)_{dCO}(H_2O)_4]^1$	Al-O_C	1.827	0.198	0.0787	0.5040	-0.0030
		Al-O	1.766	0.245	0.0951	0.6240	-0.0091
		Al-O_{W1}	1.984	0.124	0.0504	0.2935	0.0012
		Al-O_{W2}	1.961	0.126	0.0522	0.3166	0.0018
		Al-O_{W3}	1.994	0.125	0.0497	0.2924	0.0017
		Al-O_{W4}	1.994	0.122	0.0486	0.2830	0.0017
	$[Al(Ser)_{dCN}(H_2O)_4]^1$	Al-O_C	1.811	0.208	0.0794	0.5939	0.0046
		Al-N	2.000	0.176	0.0620	0.3189	-0.0045
		Al-O_{W1}	1.974	0.127	0.0482	0.3084	0.0043
		Al-O_{W2}	1.958	0.134	0.0509	0.3290	0.0044
		Al-O_{W3}	1.930	0.134	0.0526	0.3643	0.0067
		Al-O_{W4}	1.934	0.138	0.0533	0.3561	0.0051
		H_{W2}-H	1.655	0.047	0.0217	0.0435	-0.0013
	$[Al(Ser)_{tCNO}(H_2O)_4]^1$	Al-O_C	1.880	0.181	0.0717	0.4193	-0.0042
		Al-O	1.803	0.226	0.0882	0.5496	-0.0084
		Al-N	2.048	0.151	0.0569	0.2471	-0.0076
		Al-O_{W1}	1.971	0.133	0.0517	0.3053	0.0014
		Al-O_{W2}	1.958	0.136	0.0538	0.3198	0.0014
		Al-O_{W3}	1.952	0.136	0.0536	0.3264	0.0019

Table S5: Distance (in Å) and electron delocalitation indexes (DI) of the first coordination sphere of aluminum and of hydrogen bonds in representative Al-PSer structures. QTAIM parameters of *Al...O* and *Al...N* bond critical points (BCP, in au): ρ_{BCP}, the electron density at BCP; ∇^2_{BCP}, the laplacian of the electron density; and H_{BCP}, the total electron energy density at BCP. O_C stands for carboxylate group oxygen atom, and O_P for phosphate group oxygen atom. The subscripts indicate the coordination mode of PSer to Al^{3+}.

$Al^{3+} - PSer$ Complexes

Titrable groups	Structure	Distance		DI	ρ_{BCP}	∇^2_{BCP}	H_{BCP}
NH_3^+, COO^-, $OHPO_3^-$	$[Al(PSer)_{mC}(H_2O)_5]^2$	Al-O_C	1.844	0.178	0.0737	0.4691	-0.0017
		Al-O_{W1}	1.876	0.172	0.0688	0.4236	-0.0012
		Al-O_{W2}	1.921	0.152	0.0605	0.3632	0.0000
		Al-O_{W3}	1.936	0.140	0.0569	0.3447	0.0012
		Al-O_{W4}	1.946	0.142	0.0563	0.3328	0.0006
		Al-O_{W5}	1.930	0.140	0.0571	0.3514	0.0016
		H_{W1}-O_P	1.428	0.186	0.0894	0.1163	-0.0339
		H_{W2}-O_C	1.689	0.113	0.0480	0.1185	-0.0065
		H_{W4}-O_P	1.722	0.098	0.0416	0.1150	-0.0036
		H_N-H_P	1.793	0.115	0.0384	0.1063	-0.0024
	$[Al(PSer)_{dCP}(H_2O)_4]^2$	Al-O_C	1.865	0.169	0.0690	0.4352	-0.0008
		Al-O_P	1.823	0.189	0.0762	0.5068	-0.0010
		Al-O_{W1}	1.948	0.135	0.0547	0.3298	0.0014
		Al-O_{W2}	1.952	0.133	0.0545	0.3264	0.0013
		Al-O_{W3}	1.934	0.143	0.0580	0.3481	0.0007
		Al-O_{W4}	1.939	0.150	0.0588	0.3407	-0.0005
		H_{W4}-O_C	1.686	0.112	0.0477	0.1225	-0.0061
		H_{W3}-O_P	1.797	0.079	0.0334	0.1128	0.0000
NH_3^+, COO^-, OPO_3^{-2}	$[Al(PSer)_{dCP}(H_2O)_4]^1$	Al-O_C	1.843	0.176	0.0714	0.4691	-0.0001
		Al-O_P	1.815	0.204	0.0804	0.5220	-0.0034
		Al-O_{W1}	1.989	0.125	0.0502	0.2880	0.0009
		Al-O_{W2}	1.969	0.129	0.0526	0.3082	0.0009

Table S5: Distance (in Å) and electron delocalitation indexes (DI) of the first coordination sphere of aluminum and of hydrogen bonds in representative Al-PSer structures. QTAIM parameters of *Al...O* and *Al...N* bond critical points (BCP, in au): ρ_{BCP}, the electron density at BCP; ∇^2_{BCP}, the laplacian of the electron density; and H_{BCP}, the total electron energy density at BCP. O_C stands for carboxylate group oxygen atom, and O_P for phosphate group oxygen atom. The subscripts indicate the coordination mode of PSer to Al^{3+}.

		Al-O_{W3}	1.912	0.161	0.0630	0.3730	-0.0009
		Al-O_{W4}	1.967	0.129	0.0525	0.3100	0.0013
		H_{W3}-O_P	1.444	0.188	0.0882	0.1210	-0.0324
		H_N-O_P	1.756	0.119	0.0417	0.1186	-0.0029
NH_2, COO^-, OPO_3^{-2}	$[Al(PSer)_{tCP}(H_2O)_3]$	Al-O_C	1.825	0.190	0.0763	0.5026	-0.0015
		Al-O_P	1.875	0.188	0.0727	0.4299	-0.0050
		Al-O_P	1.888	0.181	0.0702	0.4121	-0.0045
		Al-O_{W1}	2.020	0.114	0.0458	0.2588	0.0012
		Al-O_{W2}	1.978	0.130	0.0516	0.2993	0.0010
		Al-O_{W3}	1.946	0.137	0.0551	0.3339	0.0016
		H_N-O_P	2.187	0.055	0.0166	0.0570	0.0014
	$[Al(PSer)_{tCNP}(H_2O)_3]$	Al-O_C	1.867	0.199	0.0740	0.4368	-0.0047
		Al-O_P	1.803	0.229	0.0845	0.5447	-0.0055
		Al-N	2.116	0.132	0.0499	0.2002	-0.0066
		Al-O_{W1}	1.989	0.130	0.0495	0.2869	0.0014
		Al-O_{W2}	1.983	0.133	0.0516	0.2921	0.0006
		Al-O_{W3}	2.051	0.116	0.0448	0.2320	-0.0008
		O_{W3}-H	2.610	0.028	0.0094	0.0311	0.0009
		H_{W3}-O_P	1.432	0.198	0.0918	0.1171	-0.0356
		N-O_P	2.595	0.072	0.0218	0.1017	0.0035

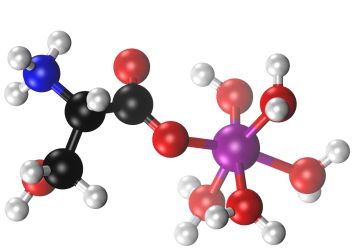
$[Al(OH)]^{2+}$species

Table S6: Enthalpy and free energy affinities in kcal/mol for $[Al(OH)]^{2+} - Ser$ complexes formation with corrections that account for the physiological pH and deprotonation of the corresponding titratable groups.

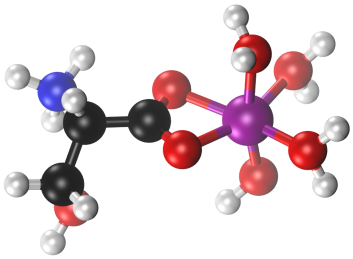
$[Al(OH)]^{2+} - Ser$ **Complexes**

Titratable groups	Structure	ΔH_{aq}^{compl}	ΔG_{aq}^{compl}	ΔG_{aq}^{Phys}
NH_3^+, COO^-, OH	$[Al(Ser)_{mC}(H_2O)_4(OH)]^2$	-19.67	-15.34	-15.34
	$[Al(Ser)_{bC}(H_2O)_3(OH)]^2$	-2.95	-5.99	-5.99
NH_3^+, COO^-, O^-	$[Al(Ser)_{mC}(H_2O)_4(OH)]^1$	-30.44	-23.98	-16.34
	$[Al(Ser)_{bC}(H_2O)_3(OH)]^1$	-12.04	-14.59	-6.95
	$[Al(Ser)_{O}(H_2O)_4(OH)]^1$	-54.79	-48.54	-40.90
	$[Al(Ser)_{O}(H_2O)_4(OH)]^1$	-55.21	-48.32	-40.68
	$[Al(Ser)_{dCO}(H_2O)_3(OH)]^1$	-55.91	-58.27	-50.63
NH_2, COO^-, OH	$[Al(Ser)_{mC}(H_2O)_4(OH)]^1$	-34.14	-27.90	-25.65
	$[Al(Ser)_{mC}(H_2O)_4(OH)]^1$	-28.47	-23.32	-21.07
	$[Al(Ser)_{mC}(H_2O)_4(OH)]^1$	-31.58	-24.02	-21.77
	$[Al(Ser)_{bC}(H_2O)_3(OH)]^1$	-17.20	-19.65	-17.40
	$[Al(Ser)_{N}(H_2O)_4(OH)]^1$	-23.47	-16.99	-14.74
	$[Al(Ser)_{dCN}(H_2O)_3(OH)]^1$	-29.95	-32.53	-30.27
NH_2, COO^-, O^-	$[Al(Ser)_{mC}(H_2O)_4(OH)]$	-42.97	-37.09	-27.20
	$[Al(Ser)_{bC}(H_2O)_3(OH)]$	-27.68	-30.92	-21.03
	$[Al(Ser)_{O}(H_2O)_4(OH)]$	-64.69	-57.16	-47.27
	$[Al(Ser)_{dCO}(H_2O)_3(OH)]$	-68.21	-70.53	-60.64
	$[Al(Ser)_{dCN}(H_2O)_3(OH)]$	-39.14	-40.20	-30.30
	$[Al(Ser)_{tCNO}(H_2O)_2(OH)]$	-68.37	-77.13	-67.24

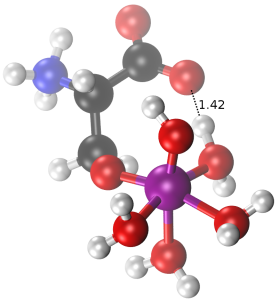
Figure S2: Representative structures of $[Al(OH)]^{2+} - Ser$ complexes. The complexation free energies for the physiological pH (ΔG_{aq}^{Phys}) and ΔH_{aq}^{compl} are shown in kcal/mol ($\Delta G_{aq}^{Phys}/\Delta H_{aq}^{compl}$). The subscripts indicate the coordination mode of Ser to $[Al(OH)]^{2+}$.



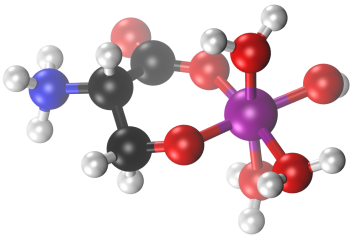
a) $[Al(Ser)_{mC}(H_2O)_4(OH)]^2$
-15.34/-19.67



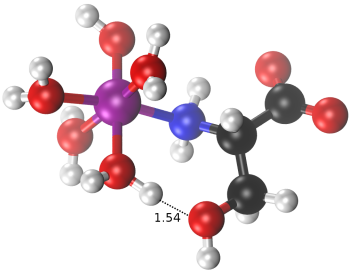
b) $[Al(Ser)_{bC}(H_2O)_3(OH)]^2$
-5.99/-2.95



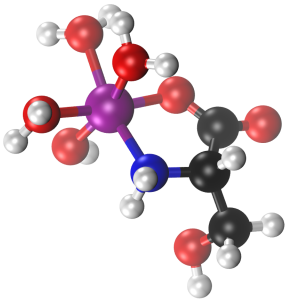
c) $[Al(Ser)_{O}(H_2O)_4(OH)]^1$
–40.90/-54.79



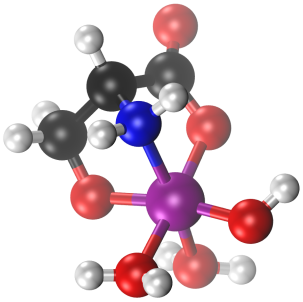
d) $[Al(Ser)_{dCO}(H_2O)_3(OH)]^1$
-50.63/-55.91



e) $[Al(Ser)_{N}(H_2O)_4(OH)]^1$
-14.74/-23.47



f) $[Al(Ser)_{dCN}(H_2O)_3(OH)]^1$
-30.27/-29.95



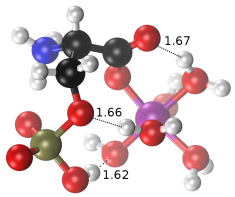
g) $[Al(Ser)_{tCNO}(H_2O)_2(OH)]$
-67.24/-68.37

Table S7: Enthalpy and free energy affinities in kcal/mol for $[Al(OH)]^{2+} - PSer$ complexes formation with corrections that account for the physiological pH and de/protonation of the corresponding titratable groups. The † sign indicates a spontaneous proton transfer from a water molecule to the phosphate group during the geometry optimization. The § sign indicates a spontaneous proton transfer from amine to phosphate group during the optimization.

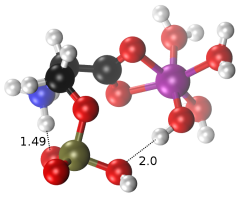
$[Al(OH)]^{2+} - PSer$ **Complexes**

Titratable groups	Structure	ΔH_{aq}^{compl}	ΔG_{aq}^{compl}	ΔG_{aq}^{Phys}
NH_3^+, COO^-, $OHPO_3^-$	$[Al(PSer)_{mC}(H_2O)_4(OH)]^1$	-36.20	-25.27	-23.06
	$[Al(PSer)_{mC}(H_2O)_4(OH)]^1$	-33.70	-23.30	-21.09
	$[Al(PSer)_{mC}(H_2O)_4(OH)]^1$	-22.08	-14.21	-12.00
	$[Al(PSer)_{bC}(H_2O)_3(OH)]^1$	-9.30	-9.96	-7.75
	$[Al(PSer)_{mP}(H_2O)_4(OH)]^1$	-24.34	-18.85	-16.64
	$[Al(PSer)_{dCP}(H_2O)_3(OH)]^1$	-30.03	-29.74	-27.53
	$[Al(PSer)_{dCP}(H_2O)_3(OH)]^1$	-27.55	-27.39	-25.18
NH_3^+, COO^-, OPO_3^{-2}	$[Al(PSer)_{mC}(H_2O)_4(OH)]$ (§)	-65.43	-54.82	-54.82
	$[Al(PSer)_{mC}(H_2O)_4(OH)]$ (†)	-64.63	-54.76	-54.76
	$[Al(PSer)_{mC}(H_2O)_4(OH)]$ (†)	-62.82	-54.01	-54.01
	$[Al(PSer)_{mP}(H_2O)_4(OH)]$	-62.73	-54.93	-54.93
	$[Al(PSer)_{bP}(H_2O)_3(OH)]$	-54.23	-54.46	-54.46
	$[Al(PSer)_{bP}(H_2O)_3(OH)]$	-56.27	-55.33	-55.33
	$[Al(PSer)_{bP}(H_2O)_3(OH)]$	-56.16	-56.46	-56.46
	$[Al(PSer)_{bP}(H_2O)_3(OH)]$	-59.88	-59.97	-59.97
	$[Al(PSer)_{dCP}(H_2O)_3(OH)]$	-61.45	-60.18	-60.18
	$[Al(PSer)_{dCP}(H_2O)_3(OH)]$	-69.06	-65.98	-65.98
	$[Al(PSer)_{tCP}(H_2O)_2(OH)]$	-54.69	-62.06	-62.06
NH_2, COO^-, OPO_3^{-2}	$[Al(PSer)_{mC}(H_2O)_4(OH)]^-$	-30.76	-25.57	-22.23
	$[Al(PSer)_{N}(H_2O)_4(OH)]^-$ (†)	-82.07	-70.75	-67.41
	$[Al(PSer)_{N}(H_2O)_4(OH)]^-$ (†)	-63.74	-54.09	-50.74
	$[Al(PSer)_{N}(H_2O)_4(OH)]^-$	-44.35	-34.00	-30.66
	$[Al(PSer)_{mP}(H_2O)_4(OH)]^-$ (†)	-64.41	-56.56	-53.21
	$[Al(PSer)_{mP}(H_2O)_4(OH)]^-$ (†)	-62.92	-55.09	-51.74
	$[Al(PSer)_{bP}(H_2O)_3(OH)]^-$	-51.73	-52.48	-49.14
	$[Al(PSer)_{dCP}(H_2O)_3(OH)]^-$	-78.49	-75.04	-71.69
	$[Al(PSer)_{tCP}(H_2O)_2(OH)]^-$	-58.34	-65.61	-62.27
	$[Al(PSer)_{tCNP}(H_2O)_2(OH)]^-$	-42.24	-47.80	-44.46
	$[Al(PSer)_{tCNbP}(H_2O)(OH)]^-$	-52.36	-67.01	-63.67

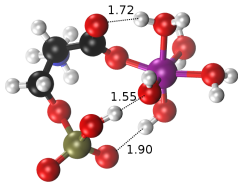
Figure S3: Representative structures of $[Al(OH)]^{2+} - PSer$ complexes. The $\Delta G_{aq}^{Phys}/\Delta H_{aq}^{compl}$ are shown in kcal/mol. The subscripts indicate the coordination mode of PSer to $[Al(OH)]^{2+}$. The † sign indicates a spontaneous proton transfer from a water molecule to phosphate group during the optimization. While the ‡ sign indicates two spontaneous proton transfer from a water molecule to the phosphate group and from another water molecule to carboxylate group during the optimization.



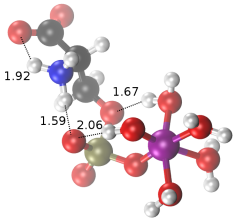
a) $[Al(PSer)_{mC}(H_2O)_4(OH)]^1$
-23.06/-36.20



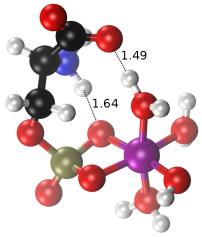
b) $[Al(PSer)_{bC}(H_2O)_3(OH)]^1$
-7.55/-9.30



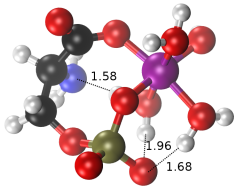
c) $[Al(PSer)_{mC}(H_2O)_4(OH)]^1$ (†)
-54.76/-64.63



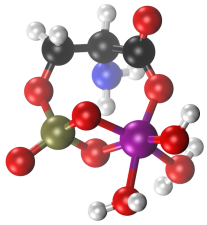
d) $[Al(PSer)_{mP}(H_2O)_4(OH)]$
-54.93/-62.73



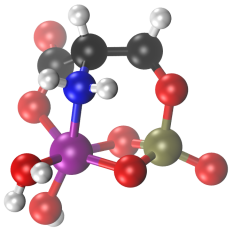
e) $[Al(PSer)_{bP}(H_2O)_3(OH)]$
-59.97/-59.88



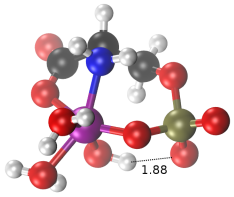
f) $[Al(PSer)_{dCP}(H_2O)_3(OH)]^{-1}$
-71.69/-78.49



g) $[Al(PSer)_{tCP}(H_2O)_2(OH)]^{-1}$
-62.27/-58.34



h) $[Al(PSer)_{tCNbP}(H_2O)(OH)]^{-1}$
-63.67/-52.36



i) $[Al(PSer)_{tCNP}(H_2O)_2(OH)]^{-1}$
-44.46/–42.24

Table S8: Distance (in Å) and electron delocalization indexes (DI) of aluminum interactions with the functional groups in representative $[Al(OH)]^{2+} - Ser/PSer$ structures. QTAIM parameters of $Al...O$ and $Al...N$ bond critical points (BCP, in au): $\rho(r_{BCP})$, the electron density at BCP; $\nabla^2\rho(r_{BCP})$, the laplacian of the electron density; and $H(r_{BCP})$, the total electron energy density at BCP. O_C stands for carboxylate group oxygen atom, O_P for phosphate group oxygen atom, O for alkoxide oxygen atom, O_H for hydroxy group oxygen atom, and O_W for average water oxygen. The subscripts indicate the coordination mode of Ser/PSer to $[Al(OH)]^{2+}$.

Titratable groups	Structure	Distance		DI	$\rho(r_{BCP})$	$\nabla^2\rho(r_{BCP})$	$H(r_{BCP})$
NH_3^+, O^-	$[Al(Ser)_{dCO}(H_2O)_3(OH)]^1$	Al-O_C	1.899	0.161	0.0631	0.3898	0.0004
		Al-O	1.815	0.213	0.0832	0.5251	-0.0058
		Al-O_H	1.793	0.239	0.0896	0.5653	-0.0084
		Al-O_W	2.022	0.112	0.0447	0.2575	0.0019
	$[Al(Ser)_O(H_2O)_4(OH)]^1$	Al-O	1.790	0.224	0.0862	0.5707	-0.0047
		Al-O_H	1.790	0.243	0.0900	0.5738	-0.0079
		Al-O_W	2.005	0.121	0.0484	0.2776	0.0010
NH_2, O^-	$[Al(Ser)_{dCO}(H_2O)_3(OH)]$	Al-O_C	1.872	0.175	0.0686	0.4287	-0.0007
		Al-O	1.803	0.220	0.0861	0.5473	-0.0067
		Al-O_H	1.796	0.237	0.0890	0.5596	-0.0084
		Al-O_W	2.041	0.107	0.0429	0.2422	0.0017
	$[Al(Ser)_{dCN}(H_2O)_3(OH)]$	Al-O_C	1.848	0.197	0.0758	0.4694	-0.0034
		Al-N	2.048	0.158	0.0584	0.2449	-0.0086
		Al-O_H	1.781	0.248	0.0925	0.5916	-0.0091
		Al-O_W	2.004	0.121	0.0472	0.2724	0.0016
	$[Al(Ser)_{tCNO}(H_2O)_2(OH)]$	Al-O_C	1.931	0.159	0.0617	0.3504	-0.0021
		Al-O	1.845	0.203	0.0788	0.4733	-0.0061
		Al-N	2.094	0.134	0.0502	0.2166	-0.0054
		Al-O_H	1.794	0.244	0.0891	0.5658	-0.0079
		Al-O_W	2.009	0.117	0.0463	0.2701	0.0020
NH_3^+, OPO_3^{-2}	$[Al(PSer)_{dCP}(H_2O)_3(OH)]$	Al-O_C	1.879	0.164	0.0665	0.4144	-0.0007
		Al-O_P	1.839	0.196	0.0766	0.4800	-0.0034
		Al-O_H	1.839	0.208	0.0789	0.4827	-0.0049
		Al-O_W	1.992	0.126	0.0500	0.2860	0.0008
NH_2, OPO_3^{-2}	$[Al(PSer)_{tCP}(H_2O)_2(OH)]^-$	Al-O_C	1.870	0.169	0.0664	0.4261	0.0005
		Al-O_P	1.932	0.166	0.0620	0.3518	-0.0029
		Al-O_P	1.942	0.158	0.0612	0.3414	-0.0034
		Al-O_H	1.794	0.245	0.0891	0.5658	-0.0077
		Al-O_W	2.054	0.107	0.0424	0.2322	0.0010
	$[Al(PSer)_{tCNP}(H_2O)_2(OH)]^-$	Al-O_C	1.925	0.170	0.0634	0.4577	-0.0032
		Al-O_P	1.852	0.203	0.0745	0.4577	-0.0038
		Al-N	2.128	0.129	0.0481	0.1937	-0.0060
		Al-O_H	1.837	0.228	0.0811	0.4868	-0.0070
		Al-O_W	2.056	0.115	0.0434	0.2307	0.0001

$[Al(OH)_2]^+$ species

Table S9: Enthalpy and free energy affinities in kcal/mol for $[Al(OH)_2]^+ - Ser$ complexes formation with corrections that account for the physiological pH and deprotonation of the corresponding titratable groups.

$[Al(OH)_2]^+ - Ser$ **Complexes**

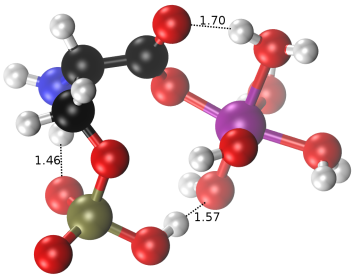
Titratable groups	Structure	ΔH_{aq}^{compl}	ΔG_{aq}^{compl}	ΔG_{aq}^{Phys}
NH_3^+, COO^-, OH	$[Al(Ser)_{mC}(H_2O)_3(OH)_2]^1$	-10.64	-6.74	-6.74
	$[Al(Ser)_{bC}(H_2O)_2(OH)_2]^1$	0.28	-2.98	-2.98
NH_3^+, COO^-, O^-	$[Al(Ser)_{mC}(H_2O)_3(OH)_2]$	-22.94	-16.09	-8.44
	$[Al(Ser)_{bC}(H_2O)_2(OH)_2]$	-6.28	-9.51	-1.87
	$[Al(Ser)_{O}(H_2O)_3(OH)_2]$	-33.80	-28.68	-21.04
	$[Al(Ser)_{dCO}(H_2O)_2(OH)_2]$	-35.20	-37.13	-29.49
NH_2, COO^-, OH	$[Al(Ser)_{mC}(H_2O)_3(OH)_2]$	-24.00	-19.36	-17.11
	$[Al(Ser)_{mC}(H_2O)_3(OH)_2]$	-17.00	-13.35	-11.10
	$[Al(Ser)_{bC}(H_2O)_2(OH)_2]$	-10.89	-14.45	-12.20
	$[Al(Ser)_{N}(H_2O)_3(OH)_2]$	-15.86	-9.82	-7.57
	$[Al(Ser)_{dCN}(H_2O)_2(OH)_2]$	-20.17	-22.96	-20.71
NH_2, COO^-, O^-	$[Al(Ser)_{mC}(H_2O)_3(OH)_2]^{-1}$	-22.16	-18.70	-8.81
	$[Al(Ser)_{bC}(H_2O)_2(OH)_2]^{-1}$	-16.68	-20.79	-10.89
	$[Al(Ser)_{O}(H_2O)_3(OH)_2]^{-1}$	-46.70	-40.40	-30.51
	$[Al(Ser)_{dCO}(H_2O)_2(OH)_2]^{-1}$	-44.99	-47.87	-37.97
	$[Al(Ser)_{dCN}(H_2O)_2(OH)_2]^{-1}$	-26.09	-28.79	-18.90
	$[Al(Ser)_{tCNO}(H_2O)(OH)_2]^{-1}$	-45.74	-55.01	-45.12

Table S10: Enthalpy and free energy affinities in kcal/mol for $[Al(OH)_2]^+ - PSer$ complexes formation with corrections that account for the physiological pH and de/protonation of the corresponding titratable groups.

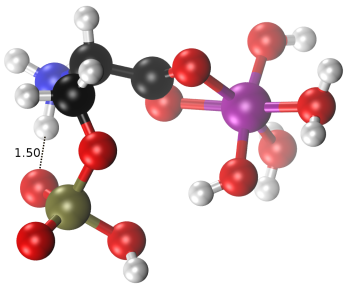
$[Al(OH)_2]^+ - PSer$ Complexes

Titratable groups	Structure	ΔH_{aq}^{compl}	ΔG_{aq}^{compl}	ΔG_{aq}^{Phys}
NH_3^+, COO^-, $OHPO_3^-$	$[Al(PSer)_{mC}(H_2O)_3(OH)_2]$	-24.46	-15.37	-13.16
	$[Al(PSer)_{bC}(H_2O)_2(OH)_2]$	-2.78	-6.01	-3.80
	$[Al(PSer)_{mP}(H_2O)_3(OH)_2]$	-14.26	-9.00	-6.79
	$[Al(PSer)_{dCP}(H_2O)_2(OH)_2]$	-11.92	-13.68	-11.47
	$[Al(PSer)_{dCP}(H_2O)_2(OH)_2]$	-13.26	-13.80	-11.59
NH_3^+, COO^-, OPO_3^{-2}	$[Al(PSer)_{mC}(H_2O)_3(OH)_2]^{-1}$	-21.24	-13.31	-13.31
	$[Al(PSer)_{mP}(H_2O)_3(OH)_2]^{-1}$	-49.09	-41.62	-41.62
	$[Al(PSer)_{mP}(H_2O)_3(OH)_2]^{-1}$	-45.26	-36.90	-36.90
	$[Al(PSer)_{bP}(H_2O)_2(OH)_2]^{-1}$	-41.91	-42.22	-42.22
	$[Al(PSer)_{dCP}(H_2O)_2(OH)_2]^{-1}$	-46.04	-43.85	-43.85
	$[Al(PSer)_{tCP}(H_2O)(OH)_2]^{-1}$	-35.47	-42.10	-42.10
NH_2, COO^-, OPO_3^{-2}	$[Al(PSer)_{mC}(H_2O)_3(OH)_2]^{-2}$	-30.79	-22.02	-18.67
	$[Al(PSer)_{mC}(H_2O)_3(OH)_2]^{-2}$	-25.30	-20.28	-16.94
	$[Al(PSer)_{N}(H_2O)_3(OH)_2]^{-2}$	-35.07	-26.61	-23.27
	$[Al(PSer)_{N}(H_2O)_3(OH)_2]^{-2}$	-34.29	-26.61	-23.27
	$[Al(PSer)_{mP}(H_2O)_3(OH)_2]^{-2}$	-35.46	-27.53	-24.19
	$[Al(PSer)_{bP}(H_2O)_2(OH)_2]^{-2}$	-32.34	-34.71	-31.37
	$[Al(PSer)_{dCP}(H_2O)_2(OH)_2]^{-2}$	-50.85	-47.18	-43.83
	$[Al(PSer)_{dCP}(H_2O)_2(OH)_2]^{-2}$	-45.62	-44.07	-40.73
	$[Al(PSer)_{tCP}(H_2O)(OH)_2]^{-2}$	-32.77	-39.70	-36.36

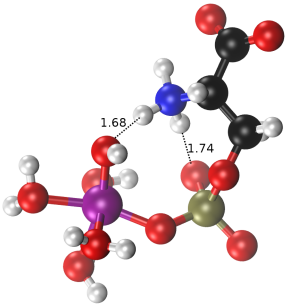
Figure S4: Representative structures of $[Al(OH)_2]^+ - PSer$ complexes. The complexation free energies for the physiological pH (ΔG_{aq}^{Phys}) and ΔH_{aq}^{compl} are shown in kcal/mol ($\Delta G_{aq}^{Phys}/\Delta H_{aq}^{compl}$). The subscripts indicate the coordination mode of PSer to $[Al(OH)_2]^{1+}$.



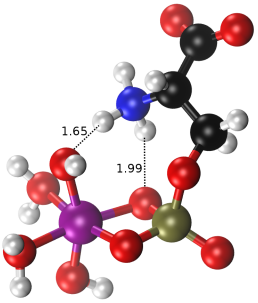
a) $[Al(PSer)_{mC}(H_2O)_3(OH)_2]$
-13.16/-24.46



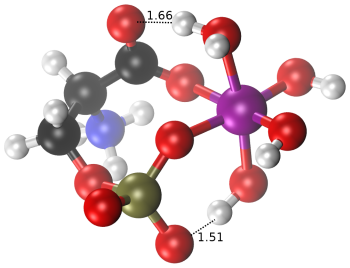
b) $[Al(PSer)_{bC}(H_2O)_2(OH)_2]$
-3.80/-2.78



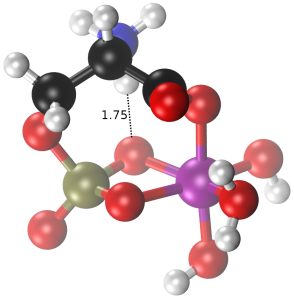
c) $[Al(PSer)_{mP}(H_2O)_3(OH)_2]^{-1}$
-41.62/-49.09



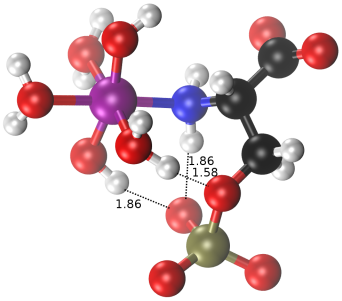
d) $[Al(PSer)_{bP}(H_2O)_2(OH)_2]^{-1}$
-42.22/-41.91



e) $[Al(PSer)_{dCP}(H_2O)_2(OH)_2]^{-1}$
-43.85/-46.04



f) $[Al(PSer)_{tCP}(H_2O)(OH)_2]^{-1}$
-42.10/-35.47



g) $[Al(PSer)_N(H_2O)_3(OH)_2]^{-2}$
-23.27/-35.07

Table S11: Distance (in Å) and electron delocalization indexes (DI) of aluminum interactions with the functional groups in representative $[Al(OH)_2]^+ - Ser/PSer$ structures. QTAIM parameters of $Al...O$ and $Al...N$ bond critical points (BCP, in au): $\rho(r_{BCP})$, the electron density at BCP; $\nabla^2\rho(r_{BCP})$, the laplacian of the electron density; and $H(r_{BCP})$, the total electron energy density at BCP. O_C stands for carboxylate group oxygen atom, O_P for phosphate group oxygen atom, O for alkoxide oxygen atom, O_H for hydroxy group oxygen atom, and O_W for average water oxygen. The subscripts indicate the coordination mode of Ser/PSer to Al^{1+}.

Titratable groups	Structure	Distance		DI	$\rho(r_{BCP})$	$\nabla^2\rho(r_{BCP})$	$H(r_{BCP})$
NH_3^+, O^-	$[Al(Ser)_{dCO}(H_2O)_2(OH)_2]$	Al-O_C	1.986	0.128	0.0497	0.2866	0.0010
		Al-O	1.849	0.196	0.0753	0.4682	-0.0033
		Al-O_H	1.820	0.227	0.0836	0.5132	-0.0070
		Al-O_H	1.843	0.211	0.0786	0.4741	-0.0055
		Al-O_W	2.098	0.097	0.0375	0.1994	0.0010
	$[Al(Ser)_O(H_2O)_3(OH)_2]$	Al-O	1.820	0.213	0.0803	0.5163	-0.0034
		Al-O_H	1.804	0.242	0.0867	0.5462	-0.0068
		Al-O_H	1.825	0.231	0.0831	0.5078	-0.0066
		Al-O_W	2.104	0.097	0.0382	0.1977	0.0003
NH_2, O^-	$[Al(Ser)_{dCO}(H_2O)_2(OH)_2]^-$	Al-O_C	1.923	0.154	0.0596	0.3581	0.0002
		Al-O	1.825	0.214	0.0805	0.5062	-0.0048
		Al-O_H	1.856	0.204	0.0760	0.4545	-0.0050
		Al-O_H	1.853	0.206	0.0768	0.4574	-0.0055
		Al-O_W	2.123	0.094	0.0359	0.1835	0.0005
	$[Al(Ser)_{dCN}(H_2O)_2(OH)_2]^-$	Al-O_C	1.895	0.170	0.0664	0.3975	-0.0016
		Al-N	2.045	0.152	0.0566	0.2497	-0.0068
		Al-O_H	1.814	0.229	0.0842	0.5251	-0.0066
		Al-O_H	1.834	0.219	0.0806	0.4908	-0.0060
		Al-O_W	2.096	0.103	0.0403	0.2204	0.0013
	$[Al(Ser)_{tCNO}(H_2O)(OH)_2]^-$	Al-O_C	1.949	0.153	0.0577	0.3280	-0.0008
		Al-O	1.903	0.179	0.0670	0.3840	-0.0034
		Al-N	2.265	0.089	0.0340	0.1281	-0.0030
		Al-O_H	1.813	0.236	0.0842	0.5276	-0.0060
		Al-O_H	1.816	0.236	0.0836	0.5211	-0.0060
		Al-O_W	2.157	0.087	0.0327	0.1634	0.0006
NH_3^+, OPO_3^{-2}	$[Al(PSer)_{dCP}(H_2O)_2(OH)_2]^-$	Al-O_C	2.049	0.105	0.0415	0.2268	0.0009
		Al-O_P	1.931	0.151	0.0581	0.3448	0.0001
		Al-O_H	1.819	0.230	0.0838	0.5142	-0.0069
		Al-O_H	1.825	0.224	0.0819	0.5035	-0.0060
		Al-O_W	2.034	0.120	0.0453	0.2461	0.0006
NH_2, OPO_3^{-2}	$[Al(PSer)_{tCP}(H_2O)(OH)_2]^{-2}$	Al-O_C	1.934	0.143	0.0556	0.3378	0.0013
		Al-O_P	2.061	0.119	0.0455	0.2275	-0.0022
		Al-O_P	1.945	0.163	0.0594	0.3326	-0.0023
		Al-O_H	1.813	0.239	0.0848	0.5259	-0.0069
		Al-O_H	1.865	0.204	0.0742	0.4383	-0.0046
		Al-O_W	2.134	0.092	0.0355	0.1764	-0.0001