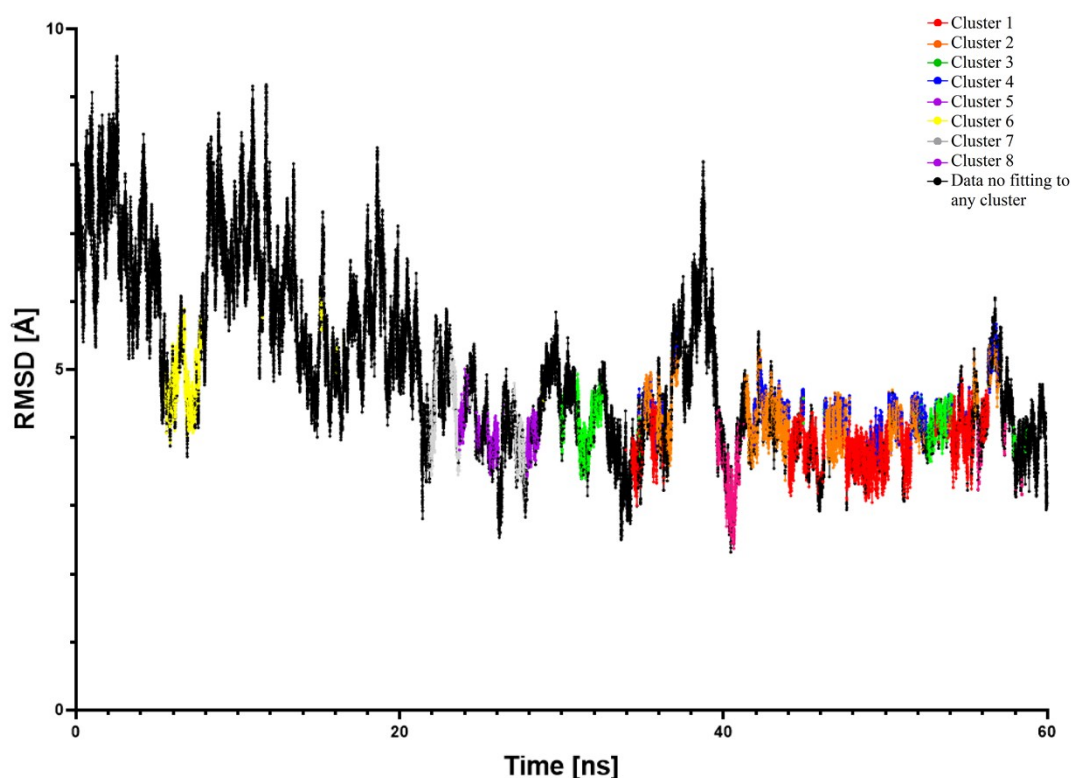


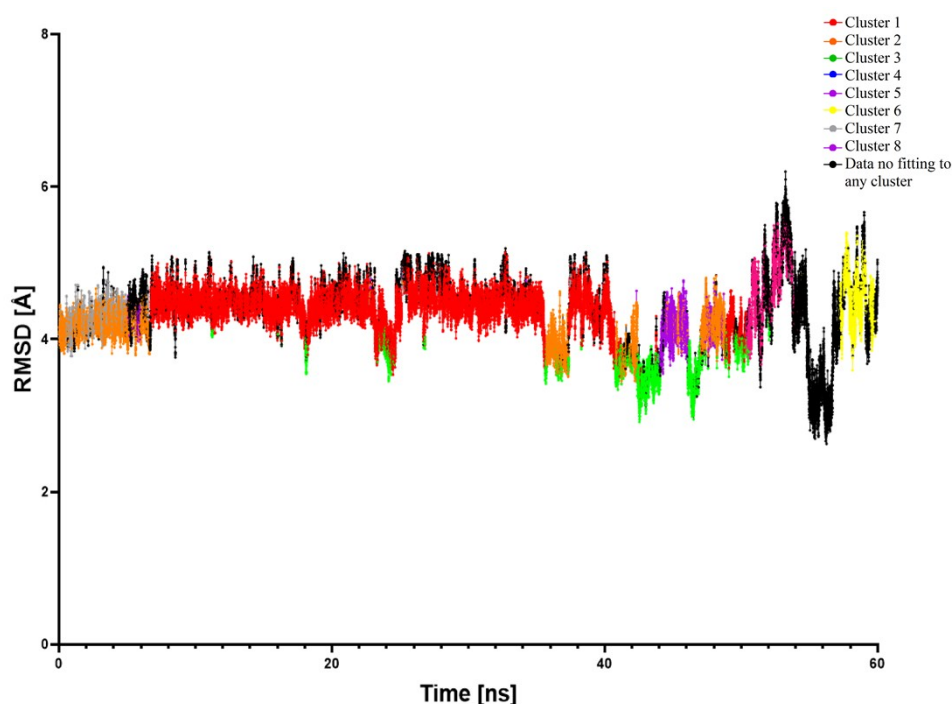
Experimental and computational studies of noncovalent interaction in the metal-free ternary  
*Lys-tn-ATP* system- Electronic Supplementary Information

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**Figure S1.** Graph representing the conformational clusters obtained by RMSD-based clustering for  $(Lys)_4(tn)(ATP)$  complex. Clusters are colored respectively Cluster 1- red, Cluster 2- orange, Cluster 3- green, Cluster 4- blue, Cluster 5- purple, Cluster 6- yellow, Cluster 7- grey, Cluster 8- magenta. Data not fitting to any cluster is colored black.



**Figure S2.** Graph representing the conformational clusters obtained by RMSD-based clustering (Lys)<sub>3</sub>(tn)(ATP) complex. Clusters are colored respectively Cluster 1- red, Cluster 2- orange, Cluster 3- green, Cluster 4- blue, Cluster 5- purple, Cluster 6- yellow, Cluster 7- grey, Cluster 8- magenta. Data not fitting to any cluster is colored black.

**Table S1.** Extended version of Table 3 with calculated energies (counterpoise energy, BSSE, sum of monomers energy, counterpoise uncorrected, corrected interaction energies in vacuum and energy, sum of monomers energy and interaction energy in water) for the studied Lys\_H4\_tn\_ATP complexes.

Lys_H4_tn_ATP complex	Vacuum					Water		
	Counterpoise corrected energy [Hartree]	BSSE energy [Hartree]	Sum of monomers [hartree]	Interaction Energy (raw) [kcal/mol]	Interaction Energy (corrected) [kcal/mol]	Energy [Hartree]	Sum of monomers [hartree]	Interaction Energy [kcal/mol]
clust1	-3389.205040	0.013527	-3388.130984	-642.5	-634.0	-3389.662999	-3389.600377	-39.3
clust2	-3390.394013	0.011035	-3389.442032	-604.3	-597.4	-3390.947925	-3390.916134	-19.9
clust3	-3389.893550	0.019364	-3388.941178	-609.8	-597.6	-3390.466196	-3390.433815	-20.3
clust4	-3390.880438	0.016275	-3389.860371	-650.3	-640.1	-3391.383833	-3391.319082	-40.6
clust5	-3391.187689	0.024488	-3390.209297	-629.3	-614.0	-3391.707855	-3391.674315	-21.0
clust6	-3389.227542	0.026645	-3388.328800	-580.7	-564.0	-3389.830209	-3389.804714	-16.0
clust7	-3391.062098	0.020459	-3390.090775	-622.4	-609.5	-3391.590411	-3391.556814	-21.1
clust8	-3391.189056	0.017020	-3390.189905	-637.7	-627.0	-3391.691254	-3391.654584	-23.0

**Table S2.** Atomic coordinates of Lys\_H4\_tn\_ATP complexes: cluster 1 and cluster 2 structures.

Lys_H4_tn_ATP complexes atomic coordinates						
Atom	Cluster 1			Cluster 2		
	x	y	z	x	y	z
N	91.65100	86.58600	78.38600	90.43400	87.30800	73.08200

C	91.14500	85.71800	77.39000	89.75100	87.72300	74.25200
C	89.83300	85.96200	77.03300	89.13000	86.68200	75.05200
N	89.05500	87.12500	77.39700	89.34800	85.27900	74.89500
C	87.90000	86.95700	76.60400	88.63600	84.76600	76.03400
N	87.89700	85.81600	75.77100	88.03900	85.72200	76.90200
C	86.94700	85.49600	74.68500	87.38800	85.51100	78.23500
O	85.85000	84.96800	74.89700	86.19400	85.17200	78.30800
C	84.99300	85.78400	75.20700	86.02500	83.98800	78.09900
C	83.56700	85.24000	75.17500	84.60900	83.47500	78.41400
O	83.27200	84.55600	76.14200	84.14700	83.91600	79.46200
P	82.13900	84.89300	77.06000	82.88100	84.70100	79.53100
O	82.32400	86.27000	77.54300	82.94200	85.80200	78.54200
O	82.11800	83.98300	78.23400	82.75100	85.28500	80.90100
O	80.80600	84.77400	76.38700	81.67500	83.83800	79.28400
P	79.87000	84.87200	75.23400	80.92600	82.74300	78.58900
O	79.98000	83.64100	74.42900	81.32200	81.44900	79.19700
O	80.12000	86.06700	74.36900	81.17800	82.70300	77.10500
O	78.48400	84.95100	75.79100	79.45300	82.94100	78.79700
P	77.65100	84.44300	76.92200	78.40400	83.38400	79.76000
O	76.20100	84.61000	76.71100	77.04000	82.95200	79.38500
O	77.61800	85.30600	78.11400	78.05800	84.81500	79.69800
O	78.02200	83.04800	77.23200	78.77400	82.97000	81.14100
C	85.21800	86.94500	74.27900	87.14900	83.31400	78.83700
O	84.40200	87.05400	73.39500	86.79600	82.75000	79.84700
C	86.59900	86.62900	73.79300	88.04100	84.49500	79.10400
O	86.61200	86.28900	72.66100	88.03600	84.82900	80.26000
C	89.15900	85.18400	75.99500	88.38400	86.97600	76.31200
N	89.81200	84.04000	75.41800	88.13300	88.31500	76.69400
C	91.11300	83.80600	75.90200	88.70300	89.28400	75.78300
N	91.81800	84.55000	76.86800	89.48600	89.07100	74.57700
H	91.79500	86.65800	78.75300	90.83300	87.38800	72.84100
H	91.92200	86.84300	78.58600	90.34500	87.04700	72.65100
H	87.14800	87.61500	76.54100	88.59700	83.80400	76.28500
H	87.44000	84.76900	74.14200	87.38100	86.44500	78.67000
H	85.27900	86.12700	76.15200	86.28500	83.87100	77.08600
H	82.90600	86.05300	75.09500	83.97900	83.71100	77.60800
H	83.45000	84.68300	74.29800	84.64200	82.42800	78.45100
H	85.16900	87.78500	74.85100	87.55700	82.64700	78.18200
H	84.16000	87.39400	73.35000	86.69300	82.35600	79.86100
H	87.27200	87.34600	73.73800	89.06800	84.38000	78.96200
H	86.81000	86.58700	72.34300	88.11700	85.04000	80.41500
H	91.60800	83.02300	75.52300	88.52700	90.18200	76.01000
N	79.32900	87.43600	77.38900	79.75600	85.76800	77.72000
C	79.69900	88.76300	77.94300	79.62200	87.10700	77.15000
C	80.68700	88.67200	79.03900	80.86800	87.93700	77.23700
C	81.00200	90.02700	79.61400	80.60000	89.30200	76.64600

C	81.89500	89.89000	80.78900	81.82400	90.16800	76.77800
C	82.21100	91.19300	81.48500	81.64900	91.54600	76.19300
N	83.12000	90.98700	82.58800	82.91600	92.31200	76.28300
C	81.04900	91.82700	82.08100	80.62700	92.34900	76.90800
O	80.94600	91.48900	83.21200	81.18300	93.07500	77.69600
O	80.74700	92.75500	81.51700	79.58100	92.35300	76.39800
H	78.99100	86.85600	78.05800	80.00900	85.77600	78.64900
H	78.67900	87.45400	76.68100	78.94000	85.21800	77.64900
H	80.07600	89.29900	77.16400	79.35100	86.98200	76.17600
H	78.84300	89.17900	78.29800	78.84500	87.57100	77.65100
H	80.28800	88.09300	79.76800	81.12200	88.03700	78.23200
H	81.53500	88.22800	78.69300	81.63300	87.47900	76.72700
H	81.42900	90.63300	78.91300	80.35200	89.20600	75.63600
H	80.13200	90.45700	79.93300	79.82400	89.76500	77.16000
H	82.76200	89.46300	80.46400	82.59700	89.68400	76.27700
H	81.46400	89.26000	81.46200	82.11600	90.26400	77.78100
H	82.65700	91.83000	80.82100	81.40000	91.45000	75.17000
H	83.34000	91.81100	83.08100	82.81000	93.21800	75.92600
H	83.93400	90.58400	82.30900	83.65000	91.87800	75.80800
H	82.76100	90.39800	83.24300	83.20900	92.44200	77.21600
H	80.07700	86.97000	77.03100	80.45700	85.27100	77.28300
C	76.31900	82.68700	80.96100	72.86300	84.93700	77.49400
C	75.32300	82.72100	81.38200	73.59300	85.41300	76.55300
C	74.46500	81.96700	82.15800	73.47800	86.10800	75.61600
N	73.45600	81.97200	82.60300	74.20600	86.58500	74.66500
N	77.17900	83.42800	80.13900	73.00200	84.25400	78.50400
H	76.21000	82.23100	80.75600	72.52000	84.65300	77.10700
H	76.55500	82.59000	81.39800	72.55000	85.32000	77.87900
H	75.10100	82.82600	80.92800	73.88800	85.03600	76.13400
H	75.43500	83.17400	81.56700	73.92600	85.65700	76.96700
H	74.68000	81.86800	82.61200	73.18000	86.49100	76.02100
H	74.33300	81.50300	81.96500	73.17300	85.89400	75.17600
H	72.91100	81.48300	83.10300	74.13000	87.00400	74.07300
H	73.52000	82.38400	82.81000	74.50000	86.81900	75.00700
H	77.82300	83.40100	79.84500	72.50700	83.93000	79.10500
H	77.00800	83.55600	79.69600	73.30500	83.85100	78.23900
H	77.33700	83.88800	80.25200	73.30200	84.47200	78.93100
H	73.18900	82.06400	82.22200	74.53800	86.28900	74.22100

**Table S3.** Atomic coordinates of Lys\_H4\_tn\_ATP complexes: cluster 3, cluster 4 and cluster 5 structures.

Lys H4 tn ATP complexes atomic coordinates									
Atom	Cluster 3			Cluster 4			Cluster 5		
	x	y	z	x	y	z	x	y	z
N	91.74000	87.57700	75.38300	91.46100	88.82900	76.83500	89.99500	87.71000	73.97400
C	91.00400	86.69600	76.24400	90.61000	87.79300	77.32900	89.99400	86.74900	74.98800

C	90.11700	85.85300	75.57400	89.88400	87.15700	76.31500	89.23800	85.78800	74.93500
N	89.70700	85.95700	74.22200	89.58900	87.63100	74.94600	88.31100	85.64000	73.98300
C	88.61100	85.05400	74.17700	88.56200	86.75500	74.51900	87.72200	84.43100	74.36200
N	88.26100	84.42700	75.38300	88.21800	85.74800	75.44300	88.17400	83.82800	75.49200
C	87.08400	83.54600	75.69600	87.26000	84.65600	75.27100	87.59700	82.68400	76.25800
O	85.93900	84.01600	75.76100	86.05700	84.66600	75.54300	86.64000	82.86500	77.01500
C	85.43600	84.16200	74.66300	85.38200	84.05800	74.75500	85.57900	82.82400	76.44600
C	83.94000	84.50600	74.68200	83.96200	83.68300	75.17800	84.36500	82.81300	77.37700
O	83.29700	83.85100	75.50100	83.86200	83.56200	76.39300	84.18900	83.93600	77.84900
P	82.51500	84.47100	76.62200	82.87900	84.34000	77.21100	82.90700	84.70600	77.67900
O	83.38800	85.41100	77.37400	82.93600	85.75700	76.80700	82.45700	84.66600	76.25900
O	82.05500	83.38300	77.55200	83.25000	84.27800	78.67100	83.13400	86.13700	78.08500
O	81.30000	85.19200	76.12400	81.50100	83.76100	77.01300	81.82500	84.16000	78.56400
P	80.58200	86.06300	75.14200	80.44400	83.12300	76.17500	81.08400	83.06000	79.25700
O	80.14200	85.21500	73.99800	80.75700	81.68300	76.11900	81.79600	82.68600	80.50800
O	81.40800	87.21800	74.62300	80.35800	83.69600	74.77300	80.91400	81.85000	78.38400
O	79.36800	86.60900	75.82900	79.10700	83.30300	76.84700	79.71800	83.58400	79.59300
P	78.27400	86.24900	76.79000	78.43700	83.34400	78.19800	79.00600	84.82600	80.01700
O	77.13600	87.19800	76.75900	76.94300	83.29400	78.16500	77.67300	84.55300	80.59300
O	78.56600	86.51500	78.21500	78.39000	84.66200	78.84400	78.43000	85.63400	78.91800
O	77.82900	84.84100	76.56300	79.00600	82.30400	79.10600	79.87000	85.63200	80.93200
C	85.80400	82.90800	73.91000	86.21600	82.90700	74.32800	85.68500	81.66900	75.53500
O	84.88300	82.14400	73.74200	86.08900	81.94600	75.02000	85.08800	80.70500	75.89700
C	86.89900	82.38900	74.78000	87.59300	83.58100	74.34600	87.15900	81.50400	75.48100
O	86.57000	81.41400	75.38800	88.38900	82.87500	74.81800	87.50800	80.50200	75.97200
C	89.19900	84.95800	76.32800	88.97100	86.08700	76.67000	89.13200	84.67800	75.89100
N	89.38700	84.74000	77.71900	89.01600	85.49900	78.01100	89.89700	84.66100	76.97500
C	90.40500	85.54200	78.28200	89.84100	86.10700	78.93000	90.66000	85.73100	76.97400
N	91.23600	86.50800	77.63400	90.71600	87.19700	78.67500	90.76700	86.78400	76.06600
H	92.00600	87.87900	75.36300	91.74400	89.05200	76.99300	89.98600	87.98800	73.70400
H	91.96400	87.71300	75.04400	91.77000	89.09100	76.78100	89.95900	88.11200	73.79800
H	88.01800	84.90100	73.39600	88.10400	86.74500	73.61100	86.96800	84.02800	73.96400
H	87.24200	83.20500	76.66300	87.35600	84.27300	76.21700	88.31200	82.44300	76.93400
H	86.01600	84.89800	74.18600	85.38800	84.55600	73.86200	85.59700	83.64100	75.81000
H	83.86300	85.54300	74.85700	83.28900	84.44700	74.91300	83.51300	82.48300	76.84600
H	83.54900	84.36400	73.71600	83.65300	82.81200	74.67100	84.51400	82.10100	78.13600
H	86.14000	83.20300	72.99800	85.98400	82.59700	73.36600	85.30500	81.93700	74.65300
H	84.70800	82.03300	73.28200	86.21300	81.51200	75.02500	84.72000	80.57300	75.68800
H	87.74000	82.06000	74.32800	87.82000	83.97100	73.49200	87.56100	81.42100	74.60400
H	86.62200	81.18000	75.44000	88.85300	83.15300	75.06300	87.82500	80.29500	75.83900
H	90.55200	85.43200	79.23700	89.91700	85.75200	79.86600	91.19200	85.77800	77.72800
N	78.71600	89.33300	77.85100	79.55700	86.46800	76.88000	79.39600	89.50500	77.83200
C	79.35100	89.85500	79.08300	79.62300	87.93400	77.21900	79.60700	90.88200	78.31400
C	78.52400	90.82800	79.85500	80.48400	88.28200	78.40400	78.83700	91.17700	79.55000
C	79.24900	91.30900	81.08000	80.46700	89.78400	78.67100	79.11800	92.59000	80.01700
C	78.42800	92.31100	81.83700	81.17100	90.04100	79.97200	78.25100	92.87400	81.18000

C	79.07600	92.78000	83.11500	81.35100	91.52200	80.29000	78.44400	94.25900	81.75900
N	78.20400	93.68900	83.86900	82.21400	91.72600	81.49100	77.59400	94.39000	82.92500
C	80.31800	93.54100	82.87900	80.05400	92.25900	80.55100	78.04300	95.35100	80.80800
O	80.07000	94.72400	82.86500	79.92900	92.44500	81.75500	76.88200	95.62600	81.01700
O	81.25200	92.93100	83.14000	79.49500	92.63600	79.59300	78.97600	95.95000	80.40600
H	78.48900	90.03800	77.25100	79.24000	85.96600	77.65000	78.48100	89.35400	77.63400
H	79.26300	88.69000	77.35100	78.95800	86.28300	76.14900	79.89800	89.29100	77.02600
H	79.56200	89.03500	79.66400	79.99700	88.42900	76.37300	80.59900	90.96100	78.51200
H	80.21600	90.31600	78.79200	78.63800	88.20500	77.48700	79.32600	91.53500	77.57500
H	78.31100	91.63300	79.25200	80.13200	87.71900	79.22600	77.84800	91.06700	79.32200
H	77.64500	90.37000	80.12200	81.44400	87.94000	78.19100	79.10000	90.48700	80.28500
H	79.43600	90.50000	81.68100	80.99400	90.25400	77.91600	80.10600	92.70500	80.26800
H	80.12600	91.77400	80.81700	79.48600	90.11400	78.79000	78.88500	93.29600	79.28300
H	77.53400	91.85800	82.07200	82.11400	89.60700	79.94200	78.48500	92.15100	81.90600
H	78.23100	93.13000	81.24400	80.68800	89.51200	80.74100	77.26200	92.77100	80.88700
H	79.27500	91.95200	83.69700	81.86600	91.96100	79.47000	79.43500	94.37400	82.04400
H	78.60800	94.02000	84.69400	82.37000	92.68500	81.74000	77.67800	95.28200	83.31800
H	77.35400	93.28300	84.08800	83.10100	91.29600	81.40800	77.77900	93.71500	83.61500
H	77.98200	94.48500	83.37600	81.82800	91.34600	82.32900	76.66000	94.29900	82.72100
H	77.89100	88.88700	78.02500	80.43600	86.07100	76.71100	79.64700	88.85100	78.48100
C	77.87400	81.39000	80.18600	75.07300	86.41600	79.88600	78.67900	83.85000	75.31300
C	76.78000	81.26900	80.33400	73.79200	86.53800	80.44900	77.46100	84.57000	74.94800
C	76.06400	80.31200	80.47900	73.09700	87.84400	80.52400	76.88700	84.22500	73.63100
N	75.00000	80.14900	80.62900	71.77100	88.00100	81.06900	75.69700	84.94100	73.30700
N	78.61300	82.34000	80.05800	75.83800	85.19500	79.91500	79.21600	84.18600	76.65300
H	77.79300	80.93800	79.75800	75.62400	86.98700	80.33900	79.39700	84.07300	74.64500
H	78.22300	81.24300	80.60500	74.98600	86.65400	79.06800	78.50800	82.86900	75.34300
H	76.42400	81.41700	79.91300	73.86800	86.25200	81.26600	77.65300	85.53400	74.97800
H	76.86900	81.72500	80.76100	73.29800	85.98300	80.01300	76.78200	84.38700	75.64500
H	76.39200	80.17300	80.89900	72.90100	88.08600	79.70900	76.66900	83.26200	73.60900
H	75.95900	79.84700	80.06300	73.56600	88.37900	81.00600	77.51400	84.43000	72.89500
H	74.54800	79.51900	80.73700	71.31900	88.83000	81.01100	75.31400	84.72200	72.44300
H	75.04300	80.56400	81.00000	71.23100	87.44700	80.71100	75.03100	84.81900	73.94600
H	79.31700	82.41900	79.97700	76.65700	85.18700	79.58400	80.03100	83.74100	76.87500
H	78.34900	82.52100	79.65200	75.95000	84.90700	80.64100	79.39500	85.09100	76.72400
H	78.73000	82.80300	80.45000	75.40600	84.61800	79.55200	78.62100	83.99200	77.34300
H	74.63400	80.25600	80.25900	71.74100	87.81500	81.90500	75.84700	85.85600	73.29800

**Table S4.** Atomic coordinates of Lys\_H4\_tn\_ATP complexes: cluster 6, cluster 7 and cluster 8 structures.

Lys_H4_tn_ATP complexes atomic coordinates									
Atom	Cluster 6			Cluster 7			Cluster 8		
	x	y	z	x	y	z	x	y	z
N	92.31000	86.26400	74.29000	88.79700	81.16700	72.30000	91.73100	85.53200	78.21700
C	91.87700	85.19800	75.07700	88.38700	82.47100	72.65600	90.99300	84.71000	77.30400

C	90.65400	84.69200	74.72900	88.76200	82.86600	73.99200	89.93400	85.37700	76.63300
N	89.83600	85.09400	73.63100	88.99100	81.93200	75.06700	89.32300	86.62400	77.04300
C	88.75600	84.20400	73.67300	88.85000	82.74200	76.23500	88.09800	86.61900	76.28500
N	88.83900	83.28500	74.69100	88.44100	84.07200	76.01200	87.85000	85.46500	75.50400
C	87.77600	82.39200	75.20000	87.87200	85.05800	76.98700	86.64800	85.11600	74.67200
O	86.81200	82.87300	75.80800	86.73000	84.91200	77.44200	85.62500	84.63900	75.19000
C	85.92700	83.22400	75.07100	86.71800	84.11500	78.35200	84.92700	85.49500	75.71100
C	84.61700	83.58100	75.77200	85.39000	84.04100	79.10900	83.52400	85.02600	76.13700
O	84.71600	84.66000	76.32700	84.90600	85.13000	79.40900	83.55200	84.30700	77.13900
P	83.85600	85.83400	76.00000	83.55500	85.58800	78.94300	82.85900	84.65100	78.42500
O	83.86900	86.06500	74.54400	83.49500	85.45800	77.47400	83.24300	86.03000	78.83800
O	84.44900	87.02700	76.68100	83.36000	87.03200	79.29300	83.28500	83.68200	79.49500
O	82.44300	85.66600	76.48900	82.45000	84.79100	79.56500	81.36500	84.56400	78.29000
P	81.24000	84.80600	76.70800	81.85900	83.52000	80.06200	80.06000	84.73500	77.56100
O	81.46400	83.99800	77.91800	82.37400	83.26500	81.42600	79.85100	83.56100	76.66300
O	80.95700	83.89900	75.54700	82.16900	82.34200	79.18900	80.00100	86.01200	76.75900
O	80.03900	85.65600	76.94100	80.37500	83.71000	80.16400	78.96900	84.76800	78.59700
P	79.56300	86.91800	77.56000	79.32100	84.69400	80.53600	78.58300	84.17800	79.91800
O	78.13300	86.94400	77.85400	77.98200	84.11400	80.70100	77.15000	84.36000	80.24000
O	79.47500	88.01700	76.63800	78.85400	85.56300	79.46900	79.00300	84.97700	81.09100
O	80.34600	87.22700	78.74900	79.73000	85.46100	81.71300	79.01500	82.75600	80.01200
C	85.82900	82.16600	74.05700	87.94300	84.42200	79.18300	84.93400	86.64700	74.72300
O	84.88700	81.45200	74.19200	87.70400	84.96100	80.24000	83.89100	86.80000	74.11100
C	87.14700	81.50800	74.22000	88.70200	85.26700	78.20500	86.09800	86.24400	73.85900
O	87.02500	80.43100	74.65100	88.71600	86.42700	78.51700	85.76400	85.86500	72.75900
C	90.05700	83.58300	75.40500	88.31000	84.15800	74.56700	89.01000	84.61700	75.75500
N	90.67200	83.05800	76.59400	87.87000	85.17200	73.66800	89.41300	83.32000	75.26100
C	91.93600	83.62300	76.90500	87.75900	84.76400	72.30100	90.60400	82.79900	75.85000
N	92.57300	84.68700	76.22100	88.04800	83.49700	71.73300	91.43400	83.42500	76.83300
H	92.75900	86.41200	74.19000	88.94200	80.92100	72.10900	91.93400	86.04500	78.15800
H	92.54500	86.69700	74.30500	89.02600	80.91200	71.94200	92.21500	85.34600	78.62100
H	87.92800	84.25600	73.13000	88.85400	82.39300	77.18400	87.38800	87.32600	76.33800
H	88.23800	81.84600	75.93500	87.77500	85.93500	76.45200	86.96500	84.33100	74.07300
H	86.31500	84.04300	74.57200	86.97600	83.20100	77.90300	85.51000	85.81100	76.52100
H	83.82600	83.58700	75.08000	84.72200	83.49500	78.51100	82.92300	85.88900	76.28200
H	84.39700	82.85900	76.48200	85.54100	83.48800	79.98200	83.09800	84.45400	75.36000
H	85.71200	82.60500	73.19000	88.38600	83.51000	79.38900	85.11300	87.50900	75.26300
H	84.51300	81.56800	73.87100	87.82700	84.73300	80.62300	83.64400	87.04500	74.11200
H	87.68900	81.32200	73.42000	89.71700	85.12300	78.08600	86.76200	86.96100	73.59800
H	87.27700	80.06600	74.39100	89.06100	86.57700	78.85300	85.88900	85.96800	72.44900
H	92.38800	83.30700	77.71200	87.54200	85.47400	71.65400	90.92900	81.91000	75.55300
N	74.07200	94.11600	78.18300	77.31600	88.71500	75.44300	80.37100	87.14100	79.95100
C	74.57900	94.48200	79.49200	76.73700	89.98700	75.93200	80.53000	88.40200	80.70500
C	75.22200	93.41500	80.16200	77.13700	90.37100	77.31700	79.94500	89.60300	80.01300
C	75.71800	93.80800	81.49500	76.47300	91.64500	77.75000	80.12700	90.84200	80.86100
C	76.30900	92.67200	82.17500	76.80600	91.99200	79.16100	79.55400	92.03700	80.14300

C	76.93600	92.99800	83.48800	76.19100	93.27200	79.67200	79.55700	93.33200	80.93500
N	77.61800	91.88200	84.02100	76.64400	93.66200	81.00400	78.86700	94.39500	80.18100
C	75.98900	93.39700	84.49000	74.75200	93.21800	79.76300	80.90800	93.87200	81.22100
O	75.70400	92.48100	85.12100	74.43900	93.15700	80.88500	81.22200	94.66500	80.36800
O	75.95100	94.43400	84.68100	74.22400	93.39000	78.81000	81.21200	93.70900	82.26900
H	73.49400	93.42500	78.18500	77.07000	87.99500	76.00100	80.80700	87.18700	79.09300
H	73.63700	94.78400	77.74700	77.08300	88.45500	74.53900	80.73500	86.35500	80.40900
H	75.20300	95.21000	79.40400	77.02200	90.70300	75.27500	80.03700	88.26400	81.60500
H	73.81700	94.78600	80.00600	75.73600	89.87300	75.87500	81.54400	88.55400	80.86800
H	74.56800	92.67600	80.21800	76.85900	89.62600	77.94600	80.42900	89.75400	79.11200
H	75.98500	93.09100	79.62700	78.13600	90.48900	77.36100	78.94000	89.44700	79.84200
H	76.40300	94.52100	81.41700	76.74800	92.39600	77.14400	79.62700	90.68900	81.76000
H	74.96200	94.17500	82.01700	75.47200	91.51700	77.69100	81.12700	91.01300	81.06400
H	77.05500	92.30800	81.61300	77.80100	92.09600	79.22200	78.56600	91.79400	79.93500
H	75.61600	91.94900	82.25000	76.54500	91.23900	79.77500	80.05600	92.19400	79.24700
H	77.59400	93.74700	83.37000	76.45700	94.01200	79.05200	79.04200	93.19900	81.83000
H	78.05400	92.06200	84.87000	76.23600	94.47300	81.36800	78.86600	95.27400	80.63600
H	78.27200	91.53700	83.45100	77.58900	93.75300	81.04000	77.94900	94.16100	79.96000
H	77.04800	91.16500	84.17600	76.43500	93.00600	81.65600	79.29900	94.57700	79.33200
H	74.69700	93.82300	77.63600	78.25000	88.71900	75.44700	79.45400	86.94600	79.77600
C	78.57500	82.26300	78.26100	80.52800	84.70000	75.97400	75.74800	83.27900	75.38100
C	78.67100	82.03800	79.26500	80.82100	86.07700	75.76300	76.08000	81.98900	75.50500
C	78.91000	81.26700	80.35600	81.45300	86.35000	74.46300	76.52700	81.15800	74.57500
N	78.97800	81.02700	81.40400	81.78300	87.71300	74.24200	76.90200	79.87900	74.66900
N	78.28800	83.06300	77.18700	79.87600	84.41400	77.23500	75.31200	84.16800	76.27200
H	78.36300	82.03600	78.15800	81.34300	84.19500	75.95400	75.25000	83.33100	74.92900
H	78.90900	82.10300	78.36800	79.95000	84.40400	75.26400	76.30900	83.56500	75.12100
H	78.35300	82.22200	79.14800	81.39600	86.36000	76.51000	75.49300	81.72000	75.78600
H	78.89900	82.26500	79.34700	79.98700	86.55800	75.80300	76.58300	81.95300	75.99400
H	79.24700	81.08900	80.48000	80.87100	86.10100	73.71800	77.08300	81.42400	74.31300
H	78.70700	81.03800	80.29200	82.26700	85.86700	74.41600	76.02900	81.17800	74.09000
H	79.10600	80.52600	82.12200	82.21400	87.91300	73.41200	77.21700	79.33600	74.07700
H	79.14700	81.21500	81.52600	81.05800	88.25300	74.25800	77.38000	79.79300	75.11700
H	78.23500	83.21600	76.53900	79.64200	83.52900	77.36800	75.09900	85.01200	76.18100
H	77.98200	83.25300	77.03700	80.38600	84.64100	77.96000	74.75600	83.99500	76.56000
H	78.45500	83.33300	77.19200	79.11400	84.89800	77.36300	75.75700	84.16000	76.77200
H	78.69600	81.16500	81.33700	82.30500	88.01700	74.93800	76.38700	79.55300	74.92300

**Table S5.** Extended version of Table 4 with calculated energies (counterpoise energy, BSSE, sum of monomers energy, counterpoise uncorrected, corrected interaction energies in vacuum and energy, sum of monomers energy and interaction energy in water) for the studied Lys\_H3\_tn\_ATP complexes.

Lys_H3_tn _ATP complex	Vacuum					Water		
	Counterpoise corrected energy [Hartree]	BSSE energy [Hartree]	Sum of monomers [hartree]	Interaction Energy (raw) [kcal/mol]	Interaction Energy (corrected) [kcal/mol]	Energy [Hartree]	Sum of monomers [hartree]	Interaction Energy [kcal/mol]



clust1	-3390.732704	0.007855	-3389.913663	-518.9	-514.0	-3391.291846	-3391.275328	-10.4
clust2	-3390.285842	0.011776	-3389.438447	-539.1	-531.8	-3390.842364	-3390.829452	-8.1
clust3	-3390.642042	0.014019	-3389.804973	-534.1	-525.3	-3391.212143	-3391.197175	-9.4
clust4	-3390.624367	0.011640	-3389.832319	-504.3	-497.0	-3391.295515	-3391.271674	-15.0
clust5	-3390.216776	0.014726	-3389.438890	-497.4	-488.1	-3391.003874	-3390.975319	-17.9
clust6	-3390.487912	0.015019	-3389.600220	-566.5	-557.0	-3391.042765	-3391.003345	-24.7
clust7	-3390.162576	-0.136763	-3388.964608	-665.9	-751.7	-3391.090173	-3391.045504	-28.0
clust8	-3390.527662	-0.096382	-3389.347052	-680.4	-740.8	-3390.813856	-3390.780417	-21.0

**Table S6.** Atomic coordinates of Lys\_H3\_tn\_ATP complexes: structure obtained after minimization. cluster 1 and cluster 2 structures.

Lys_H3_tn_ATP complexes atomic coordinates						
Atom	Cluster 1			Cluster 2		
	x	y	z	x	y	z
N	14.44700	75.40000	66.52900	17.35500	72.50100	69.53900
C	14.51000	75.15200	67.93800	17.61800	73.81600	69.95100
C	15.61100	75.70600	68.62200	16.67500	74.76100	69.51300
N	16.43200	76.78800	68.10400	15.34900	74.49600	69.15200
C	17.15200	77.20900	69.26200	14.77500	75.79100	69.10300
N	16.83200	76.54700	70.46000	15.58700	76.84800	69.47200
C	17.16200	77.02200	71.83100	15.09600	78.14200	70.00800
O	16.44100	77.84700	72.35200	14.84000	78.22000	71.18800
C	16.29300	77.59000	73.51800	15.35300	79.17400	71.67200
C	15.77800	78.69400	74.44400	14.80900	79.62100	73.02500
O	15.10200	78.32200	75.38800	13.60300	79.54500	73.17400
P	15.44600	78.62700	76.81500	12.97500	78.66700	74.19800
O	16.87700	78.28800	77.04700	13.54300	77.29800	74.02200
O	14.59500	77.75100	77.69300	11.49900	78.60000	73.94400
O	15.26000	80.08700	77.09800	13.33000	79.12700	75.57400
P	14.43900	81.29600	77.44300	13.13900	79.98900	76.78000
O	15.17600	82.47700	76.92000	14.43000	80.06500	77.49700
O	14.29000	81.44700	78.93900	12.09200	79.43200	77.71300
O	13.10700	81.23000	76.76200	12.76000	81.35900	76.34800
P	12.02600	82.10900	76.21900	12.86200	82.78300	76.72800
O	12.11200	82.35300	74.77600	13.90100	83.51900	75.99800
O	10.78100	81.44000	75.81400	11.98100	83.68800	76.00800
O	11.80700	83.34600	77.00100	12.89500	83.01600	78.19200
C	17.40200	76.73200	74.03900	15.41900	80.24100	70.65700
O	18.29400	77.26000	74.64900	14.53700	81.03000	70.62800
C	17.73200	76.00600	72.76000	15.67400	79.39200	69.44100
O	18.88600	75.78300	72.58800	15.16500	79.75600	68.44300
C	15.77400	75.63900	70.08900	16.79400	76.20000	69.83700
N	14.93700	74.73500	70.83700	17.97800	76.67100	70.41600
C	13.95100	74.06700	70.04700	18.92200	75.65200	70.69800

N	13.68600	74.20400	68.64700	18.83000	74.26200	70.48400
H	14.38700	75.10400	66.12700	17.20600	72.26100	69.25200
H	14.27500	75.44700	66.17100	17.68800	71.96500	69.55700
H	17.73800	78.03700	69.31700	13.80500	75.97100	69.09300
H	17.91700	77.72800	71.65300	14.11000	78.14000	69.75400
H	15.46500	76.95300	73.38300	16.34700	78.90700	71.78300
H	15.05900	79.24000	73.90200	15.11000	80.60700	73.19500
H	16.58300	79.33800	74.67600	15.30800	79.04400	73.74100
H	17.07400	76.07700	74.77400	16.18900	80.89100	70.80000
H	18.28900	77.31700	75.05300	14.18100	81.07300	70.78600
H	17.12200	75.19000	72.65700	16.68700	79.21000	69.38100
H	19.02400	75.45100	72.41300	15.31200	79.91000	68.13400
H	13.37000	73.41600	70.53600	19.76500	75.96500	71.06700
N	19.06000	81.06900	78.50400	14.69900	75.76000	77.42400
C	18.35100	81.45000	77.27400	15.55700	76.92900	77.24700
C	18.89500	80.81700	76.02700	16.20800	77.00100	75.89500
C	18.14000	81.31900	74.83500	17.02100	78.23200	75.79600
C	18.68500	80.71500	73.55900	17.64900	78.36300	74.43400
C	17.94000	81.15900	72.31500	18.41800	79.63400	74.25600
N	18.35700	80.35900	71.14300	18.76900	79.80900	72.84700
C	18.05900	82.63800	72.00400	19.65600	79.68100	75.09200
O	17.02100	83.18600	71.70800	19.80600	80.67800	75.74500
O	19.16600	83.00500	71.80100	20.47600	78.88000	74.76200
H	19.98400	81.32300	78.48900	15.23300	74.95800	77.32300
H	18.65800	81.43800	79.32100	14.25400	75.74100	78.29500
H	17.35300	81.21400	77.41300	14.94200	77.74900	77.41700
H	18.45300	82.46800	77.19700	16.30700	76.86200	77.94700
H	19.89300	81.06000	75.91600	16.80600	76.15400	75.74200
H	18.81000	79.79100	76.09500	15.46100	77.03200	75.19100
H	17.13200	81.07100	74.95000	16.38700	79.05100	75.96600
H	18.22600	82.35000	74.77800	17.76800	78.22900	76.51400
H	18.57100	79.68100	73.65600	16.85900	78.37800	73.76800
H	19.70400	80.94100	73.44900	18.27600	77.55800	74.20300
H	16.93100	80.91000	72.46500	17.76200	80.41300	74.50800
H	18.23800	79.39700	71.27800	17.98500	79.83900	72.27800
H	17.91900	80.63000	70.30500	19.28800	79.91800	72.53700
H	19.07600	80.12100	78.61500	14.00700	75.70200	76.75300
C	9.75800	82.66900	73.80800	13.11900	85.94600	75.82300
C	8.29800	82.65100	74.16200	11.91300	86.77300	76.20900
C	7.94300	83.84000	74.96100	11.85500	86.89300	77.70500
N	6.53300	83.85600	75.31500	10.67500	87.63500	78.16000
N	10.24800	81.45800	73.19100	13.18400	85.47400	74.44300
H	10.55900	82.32700	74.52000	13.06000	84.83300	75.91800
H	10.00000	83.47700	73.19100	14.02600	86.41000	76.06200
H	7.72600	82.66700	73.29400	11.96300	87.71700	75.76900
H	8.06800	81.79400	74.70800	11.05500	86.29300	75.86900

H	8.13600	84.71000	74.44200	12.69300	87.37400	78.07900
H	8.47800	83.80400	75.83900	11.78200	85.94400	78.11800
H	5.95900	83.80000	74.54900	10.63400	88.51800	77.76900
H	6.28400	83.09500	75.84800	9.85100	87.20300	77.88700
H	9.82900	81.29500	72.31600	13.28100	86.20300	73.79800
H	11.22100	81.46100	73.04600	13.94400	84.85900	74.27500
H	10.05600	80.66200	73.72900	12.37600	84.99200	74.18200
H	6.27200	84.64900	75.79300	10.63800	87.75800	79.13300

**Table S7.** Atomic coordinates of Lys\_H3\_tn\_ATP complexes: cluster 3, cluster 4 and cluster 5 structures.

Lys_H3_tn_ATP complexes atomic coordinates									
Atom	Cluster 3			Cluster 4			Cluster 5		
	x	y	z	x	y	z	x	y	z
N	15.78700	72.16400	70.96500	12.60900	71.70200	67.40400	20.63600	75.69000	69.37500
C	15.27100	73.39100	70.44900	12.16800	73.02000	67.76800	19.42700	75.31600	70.03500
C	16.00200	74.58200	70.68200	13.25800	74.02500	67.78300	18.30100	76.18500	69.73600
N	17.14000	74.68200	71.58100	14.62100	73.69900	68.04500	18.43900	77.59300	69.38800
C	17.42400	76.11000	71.57900	15.18900	74.94500	68.52500	17.14000	78.13700	69.71300
N	16.56400	76.90500	70.79900	14.27200	75.97500	68.64400	16.25800	77.25600	70.34400
C	16.30300	78.35600	71.00500	14.50200	77.32600	69.21400	15.08200	77.64400	71.18600
O	15.65700	78.69000	71.97000	14.49700	77.50300	70.41200	15.22600	78.29500	72.21500
C	16.19600	79.54900	72.58100	15.32800	78.28300	70.72900	14.79800	79.39300	72.05100
C	15.38100	80.33800	73.60300	15.19500	78.96500	72.09500	14.63100	80.30700	73.25600
O	14.91800	79.66900	74.51100	15.32800	78.23200	73.06300	14.19100	79.81300	74.27500
P	15.27000	79.90100	75.94700	16.40200	78.42300	74.10100	14.94400	79.80400	75.56500
O	16.75600	79.93800	76.09100	17.73700	78.49200	73.43300	16.29200	79.23600	75.29600
O	14.71300	78.76700	76.76600	16.45100	77.22500	75.02700	14.24100	78.90600	76.53900
O	14.74500	81.23900	76.36500	16.19400	79.72800	74.82100	15.12300	81.21200	76.06100
P	13.67300	82.15800	76.87900	15.51900	80.56900	75.86800	14.58900	82.40500	76.80100
O	13.97000	83.50700	76.32300	15.65200	82.00200	75.45700	15.24100	83.62300	76.25900
O	13.68500	82.23500	78.38800	16.16800	80.35000	77.22100	14.87200	82.33100	78.27500
O	12.33500	81.72200	76.37400	14.06400	80.21800	75.93600	13.12100	82.49500	76.53900
P	10.98700	82.25800	76.01500	12.71400	80.78000	76.29600	11.92500	83.38900	76.47000
O	10.78600	82.48000	74.57500	11.91800	81.27400	75.15000	11.55400	83.92000	75.15200
O	9.92000	81.27300	75.79900	11.60700	79.79900	76.36100	10.62500	82.72100	76.30000
O	10.53600	83.39900	76.86400	12.73000	81.72600	77.45100	11.90200	84.44600	77.52500
C	16.98300	80.38400	71.63600	15.62300	79.21700	69.59800	13.57400	79.30100	71.20600
O	16.50100	81.38900	71.24200	15.05500	80.26900	69.56800	12.54600	79.36200	71.75200
C	17.38200	79.33200	70.63900	15.41500	78.26200	68.45800	13.88100	78.09200	70.42600
O	17.37700	79.67100	69.50100	14.93600	78.75500	67.46100	13.03600	77.31000	70.37100
C	15.61300	75.93400	70.24200	12.98100	75.38300	68.32400	17.00800	76.00900	70.45900
N	14.40200	76.06800	69.47500	11.64600	75.90000	68.20600	16.72600	74.72400	71.05800
C	13.73300	74.79500	69.19100	10.64000	74.89100	67.88700	17.84900	73.81500	71.10000
N	14.09100	73.46500	69.63100	10.81200	73.48800	67.64100	19.17900	74.01000	70.59400
H	15.90000	71.85000	71.06000	13.01900	71.66000	66.60200	21.27600	75.53200	69.66200
H	15.71900	71.70800	71.03200	12.09200	71.07700	67.46900	20.60400	75.81500	68.54600

H	18.04900	76.58400	72.25600	16.14000	75.09900	68.77700	16.91200	79.14000	69.73200
H	15.50300	78.53600	70.35400	13.52700	77.72500	69.12000	14.83800	76.74500	71.65900
H	16.90800	79.02400	73.12600	16.17300	77.67200	70.80700	15.48300	79.80800	71.40100
H	14.56900	80.77200	73.10600	14.23200	79.41100	72.14900	14.01600	81.10600	72.96400
H	15.99600	81.13500	73.93200	15.88600	79.76400	72.09900	15.57000	80.74500	73.41100
H	17.80000	80.77500	72.10800	16.59500	79.56500	69.60400	13.51700	80.09100	70.59600
H	16.40400	81.61400	71.28800	15.17700	80.56400	69.92800	12.36900	79.30300	71.94800
H	18.27400	78.94600	70.98700	16.27600	77.71500	68.29000	14.13100	78.39800	69.53900
H	17.77400	79.83400	69.33400	14.86900	78.70400	67.22200	12.83600	77.07400	70.33200
H	12.89100	74.84100	68.67800	9.71300	75.23500	67.74200	17.68200	72.93200	71.48300
N	18.16700	76.09700	76.69400	21.38300	81.74400	73.98500	15.37400	75.14700	75.76300
C	18.62300	77.42200	76.21800	21.57200	82.85800	74.93300	15.99100	75.98300	74.71800
C	19.13600	77.48500	74.81400	21.59300	82.41300	76.36700	17.48600	75.92500	74.69700
C	19.48800	78.90700	74.52300	21.69100	83.55000	77.32600	17.97100	76.97400	73.76000
C	20.11600	79.09600	73.17200	21.70000	83.03000	78.75000	19.46700	77.05100	73.70600
C	20.46000	80.53900	72.89200	21.83400	84.07600	79.82500	19.88600	78.17400	72.79700
N	20.86200	80.72700	71.50300	22.06700	83.49400	81.14800	21.32500	78.09500	72.49200
C	21.47200	81.10500	73.84600	20.69100	85.02500	79.88900	19.45100	79.54800	73.29500
O	21.09400	82.04200	74.49000	19.68300	84.64000	80.36500	20.12900	80.07300	74.11400
O	22.56500	80.67200	73.70300	20.98700	86.08300	79.62900	18.54600	79.99300	72.71900
H	18.90000	75.45300	76.71200	20.55600	81.26800	74.14500	15.65700	75.39700	76.66300
H	17.77700	76.12900	77.59000	21.40100	82.03100	73.04100	14.38800	75.16100	75.74200
H	17.79800	78.05200	76.31500	22.45200	83.29500	74.68100	15.57400	75.74100	73.79400
H	19.37900	77.72500	76.85500	20.79500	83.50500	74.77900	15.71200	76.94700	74.99400
H	19.98300	76.87200	74.74200	20.72500	81.90500	76.60000	17.83700	76.14800	75.65400
H	18.42000	77.15500	74.14700	22.40400	81.79500	76.47500	17.81400	74.96800	74.41500
H	18.62200	79.49500	74.59000	22.55300	84.08200	77.13500	17.59400	76.79500	72.80400
H	20.18500	79.22800	75.22500	20.90300	84.19600	77.24600	17.58700	77.90500	74.06800
H	19.42200	78.77400	72.46600	22.52500	82.39900	78.79100	19.81000	76.12100	73.33300
H	20.98100	78.51300	73.08800	20.82700	82.50800	78.91300	19.86000	77.22700	74.65400
H	19.56700	81.08100	72.97100	22.69800	84.60400	79.61500	19.43300	77.99200	71.86600
H	20.20900	80.43400	70.87000	22.82200	82.89700	81.16400	21.77900	78.32900	72.92800
H	21.10800	81.64300	71.27800	22.14200	84.13700	81.88800	21.58400	77.23100	72.08400
H	17.49800	75.71000	76.10800	22.07100	81.09100	74.06200	15.64300	74.20600	75.68800
C	8.25300	82.41100	74.23600	9.43200	81.04200	75.83600	9.01500	84.45900	75.36600
C	7.01800	82.30800	75.10200	8.60100	80.52500	76.99500	7.84000	84.14700	76.26700
C	6.95400	83.50400	75.98500	8.74700	81.42200	78.18700	7.96800	84.86500	77.54800
N	5.80100	83.45300	76.88500	7.99400	80.88700	79.35100	6.84300	84.60100	78.46600
N	8.68400	81.22800	73.50900	9.58700	80.13100	74.70700	9.14500	83.57400	74.21200
H	9.25200	82.15200	74.67100	10.54200	80.83200	75.79700	10.01400	83.97000	75.52600
H	8.22000	83.21600	73.58900	9.09900	81.97300	75.47700	9.04200	85.45900	75.04800
H	6.16500	82.26300	74.50700	7.58800	80.48300	76.73900	6.94600	84.46000	75.82400
H	7.07900	81.45600	75.68000	8.93000	79.56000	77.27000	7.79000	83.12800	76.46700
H	6.87700	84.36900	75.43500	8.39800	82.37700	77.97700	7.97700	85.88200	77.34000
H	7.79800	83.53500	76.57900	9.75400	81.44100	78.46000	8.83000	84.54600	78.02100
H	4.96700	83.37100	76.39600	7.05600	80.76100	79.15700	5.98200	84.78900	78.08000

H	5.82000	82.69800	77.48300	8.31200	80.01800	79.61800	6.76800	83.67700	78.72600
H	8.05500	80.95700	72.81700	8.72300	79.94000	74.26100	8.37400	83.67700	73.60400
H	9.55900	81.33700	73.06500	10.20200	80.48000	74.00300	9.96700	83.73100	73.67600
H	8.76200	80.45900	74.09500	9.95300	79.24700	74.97200	9.15000	82.62200	74.48600
H	5.71600	84.26100	77.42100	8.04300	81.46200	80.13900	6.89000	85.12200	79.28700

**Table S8.** Atomic coordinates of Lys\_H3\_tn\_ATP complexes: cluster 6, cluster 7 and cluster 8 structures.

Lys_H3_tn_ATP complexes atomic coordinates									
Atom	Cluster 6			Cluster 7			Cluster 8		
	x	y	z	x	y	z	x	y	z
N	13.73600	71.81600	69.34000	16.79200	72.65100	69.85400	10.40700	73.23100	67.30900
C	12.83900	72.94600	69.40100	17.24800	73.93300	70.29400	10.88800	74.55600	67.45400
C	13.23800	74.12000	68.70200	16.77300	75.03600	69.48100	12.10500	74.63000	67.79000
N	14.56200	74.35200	68.18500	15.51300	74.99300	68.76100	12.84200	73.56200	68.38100
C	14.48500	75.73300	67.75200	15.17100	76.40200	68.64600	13.89000	74.27400	68.91800
N	13.25400	76.40000	68.00300	16.07000	77.32200	69.28300	13.87600	75.68000	68.77700
C	13.16500	77.84800	68.32100	15.59800	78.63400	69.83500	14.85700	76.63800	69.35400
O	13.60000	78.27200	69.36500	14.99600	78.63200	70.89400	14.78800	77.02000	70.48500
C	14.13500	79.32400	69.20400	15.46100	79.44800	71.64100	15.85900	77.06600	70.99800
C	14.37200	80.18100	70.44600	14.61400	79.84400	72.85700	16.02600	77.90300	72.24800
O	15.25300	79.76900	71.17200	13.45500	80.14300	72.64900	15.43600	77.46700	73.20700
P	16.44600	80.57100	71.52800	12.30200	79.38100	73.22500	16.12600	77.10600	74.49100
O	16.99700	81.16000	70.28700	12.43100	77.95600	72.83800	17.29800	76.24700	74.18700
O	17.45400	79.65600	72.12200	11.00700	79.89300	72.65900	15.14600	76.33800	75.32400
O	16.06000	81.67500	72.45900	12.33700	79.43900	74.72600	16.62800	78.33900	75.18700
P	15.82900	82.16400	73.85900	12.08100	80.10400	76.05000	16.38100	79.42700	76.18200
O	14.79600	83.21800	73.79800	12.98800	79.45400	77.04200	17.08800	80.64400	75.73600
O	17.09000	82.74200	74.44300	10.63900	79.92000	76.46200	16.94000	79.03600	77.52900
O	15.35200	81.03400	74.70400	12.40800	81.55300	75.95500	14.91100	79.67500	76.22800
P	14.53800	80.63900	75.89100	12.87700	82.72300	76.76000	13.80500	80.62300	76.51200
O	13.22500	80.07700	75.57200	14.31000	83.04300	76.60300	13.25500	81.30800	75.33700
O	14.80900	79.28500	76.38000	12.78900	84.04900	76.13500	12.48000	79.99400	76.53700
O	14.52400	81.66800	76.96300	12.39800	82.71200	78.17100	14.09000	81.51500	77.67900
C	13.49500	80.02400	68.05600	16.01100	80.58700	70.84700	16.86700	77.32800	69.97200
O	12.63900	80.80600	68.29400	15.33800	81.56800	70.68600	17.20300	78.44500	69.79900
C	13.17400	78.82700	67.19400	16.49800	79.82200	69.64200	16.24200	76.57400	68.82200
O	12.15600	78.87700	66.58400	16.36200	80.36700	68.58700	16.38700	77.04200	67.73800
C	12.45400	75.38300	68.68200	17.05900	76.44700	69.91700	12.71600	75.94200	68.12500
N	11.17500	75.42600	69.34700	18.13700	76.69100	70.83400	12.15700	77.13300	67.70300
C	10.79600	74.17400	69.96200	18.71200	75.51400	71.40500	10.95400	76.93300	67.15600
N	11.54200	72.93700	70.03500	18.35800	74.15100	71.18000	10.28200	75.71900	66.98400
H	13.78700	71.29300	69.46400	16.79900	72.45500	69.20700	10.32600	72.90200	67.03700
H	13.91000	71.53400	69.30400	16.93200	72.04700	70.36600	10.03900	72.94900	67.34700
H	15.29300	76.30300	67.58100	14.23600	76.72300	68.39300	14.64600	73.83500	69.45000
H	12.19600	77.86200	68.72100	14.70000	78.80700	69.30500	14.45500	77.53200	69.03300

H	15.07400	79.05400	68.85300	16.31200	78.96200	72.01000	16.02500	76.08400	71.27600
H	13.48400	80.19900	70.99700	15.04800	80.68300	73.31300	15.64900	78.85200	72.04500
H	14.55300	81.16300	70.13300	14.71000	79.05500	73.54800	17.05100	78.02500	72.45400
H	14.15300	80.64300	67.56800	16.80600	81.06200	71.29600	17.77000	76.91400	70.20200
H	12.47600	80.97500	68.37900	14.98700	81.64300	70.99300	17.39700	78.67800	69.68900
H	14.00200	78.60000	66.62400	17.46300	79.49900	69.84300	16.50100	75.58100	68.92800
H	12.04300	78.85800	66.37200	16.28700	80.70800	68.52300	16.31000	76.81500	67.37200
H	9.92000	74.17200	70.40400	19.46800	75.64800	72.07600	10.52400	77.73500	66.83400
N	19.36800	84.00900	75.66300	14.44599	76.93719	74.38296	20.59300	81.36900	75.25300
C	19.30800	84.39000	77.08800	15.56198	76.76272	75.30903	21.03500	82.40200	76.21100
C	20.02100	83.52600	78.01300	16.89562	76.86199	74.63636	19.95100	82.95600	77.01800
C	19.77200	83.93300	79.42300	17.99517	76.62461	75.63357	20.46700	84.00100	77.96500
C	20.40100	83.05400	80.39400	19.34165	76.73804	74.98743	19.38000	84.57000	78.78000
C	20.13200	83.39700	81.82900	20.48396	76.62447	75.96630	19.87900	85.58000	79.78600
N	20.95400	82.71600	82.75100	21.74569	77.03802	75.31191	18.85800	85.91500	80.73000
C	18.75600	83.29500	82.16200	20.62761	75.26921	76.61490	20.55100	86.78400	79.19400
O	18.34200	82.25300	82.35000	20.74590	75.28212	77.82287	19.84400	87.61300	78.70400
O	18.28700	84.27700	82.36800	20.93108	74.41639	75.82762	21.71300	86.83500	79.41900
H	18.99000	83.16600	75.48500	14.46074	76.28059	73.69342	19.97200	81.67800	74.60800
H	18.94200	84.62100	75.06700	13.55722	76.90368	74.80079	21.30700	80.95500	74.76400
H	19.64600	85.32800	77.18400	15.46052	77.47726	76.04078	21.74600	81.98700	76.80200
H	18.34400	84.36400	77.32700	15.45806	75.81413	75.70310	21.46100	83.14000	75.66600
H	19.66400	82.59600	77.88700	16.96861	76.14052	73.89355	19.26500	83.37500	76.39200
H	21.00500	83.52900	77.81600	16.99884	77.80476	74.22658	19.50000	82.21100	77.54400
H	20.09300	84.86400	79.60400	17.91143	77.33736	76.38990	21.18100	83.59800	78.57400
H	18.78600	83.90400	79.57700	17.89097	75.69245	76.07296	20.93100	84.74700	77.43800
H	21.37700	83.10700	80.24100	19.36235	77.70328	74.59493	18.94600	83.80000	79.29100
H	20.09100	82.12800	80.20600	19.46076	76.04480	74.21389	18.65900	84.98600	78.18100
H	20.40800	84.33500	81.99300	20.31517	77.35038	76.70317	20.59900	85.11800	80.37500
H	20.79200	82.90200	83.69800	21.69909	77.93865	74.93374	18.30000	85.80900	80.51400
H	21.85300	82.84100	82.59500	22.49621	76.88021	75.78003	18.95500	86.56600	81.22900
H	20.25200	83.94100	75.38000	14.47908	77.78037	73.93068	20.12400	80.66800	75.68300
C	12.94500	77.70100	76.32000	14.56300	85.46600	77.32100	10.70300	81.17000	75.15600
C	13.45700	76.75600	77.37200	13.72500	86.54600	77.97000	9.48600	80.88900	75.97900
C	12.92300	77.12800	78.68200	13.35800	86.11100	79.33900	9.22600	82.01800	76.90900
N	13.41800	76.24100	79.73900	12.53100	87.12500	80.01000	8.03200	81.75900	77.70000
N	13.51800	77.56600	75.03600	14.82900	85.59800	75.90100	11.14900	80.08700	74.28500
H	13.44500	78.65200	76.15500	14.08900	84.57100	76.85500	11.74100	80.94900	75.53200
H	11.92600	77.68100	76.21500	15.46500	85.31600	77.83400	10.55800	82.00800	74.55800
H	13.16700	75.80000	77.16300	14.25700	87.44600	78.02400	8.63500	80.82500	75.37600
H	14.48400	76.77200	77.40700	12.85700	86.71100	77.41200	9.60800	80.02300	76.53600
H	11.90300	77.07000	78.68700	14.18900	85.96900	79.94700	9.07800	82.87600	76.36700
H	13.21700	78.07000	78.93500	12.80800	85.22900	79.30000	10.02600	82.08200	77.56400
H	13.24000	75.33500	79.55100	12.94900	87.99700	80.01700	7.26500	81.60800	77.13200
H	14.36400	76.28800	79.82600	11.69800	87.26600	79.53600	8.10500	80.95800	78.22700
H	13.33600	76.72300	74.63800	15.36700	86.38900	75.70400	10.48800	79.85500	73.58600

H	13.20600	78.25600	74.40600	15.31700	84.81400	75.53300	12.00100	80.30400	73.83200
H	14.47200	77.61100	75.07600	14.01100	85.69200	75.35900	11.30700	79.25700	74.78700
H	13.05400	76.41700	80.60400	12.30700	86.92300	80.93500	7.80900	82.49100	78.30000

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