

Supplementary Information

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Kinetics and Mechanistic Study of Hydrolysis of Adenosine Monophosphate Disodium Salt (AMPNa₂) in Acidic and Alkaline Media

Table S1: consisting of [NaOH], pH, and the kinetic parameters (k_{obs} , E_{app} , A_{∞} and $\sum di^2$) for alkaline hydrolysis of 0.0001 M AMPNa₂ at 60°C.

[NaOH]	pH ^b	$10^7 k_{\text{obs}}/\text{s}^{-1}$	$10^7 k_{\text{calc}}/\text{s}^{-1}$	$E_{\text{app}}/\text{M}^{-1}\text{cm}^{-1}$	A_{∞}	$\sum di^2$ ^c
0.0008	9.95	$1.20 \pm 0.10d$	0.65	$2718 \pm 78 d$	$0.857 \pm 0.007 d$	1.67×10^{-3}
0.002	10.28	1.66 ± 0.17	0.72	1482 ± 55	1.095 ± 0.004	1.89×10^{-3}
0.010	10.98	1.70 ± 0.35	1.06	1691 ± 154	0.915 ± 0.017	2.21×10^{-3}
0.020	11.18	1.98 ± 0.14	1.50	4177 ± 126	0.659 ± 0.013	2.55×10^{-3}
0.040	11.46	2.17 ± 0.10	2.36	3519 ± 73	0.743 ± 0.008	1.10×10^{-3}
0.050	11.62	1.47 ± 0.27	2.79	3216 ± 361	0.764 ± 0.038	2.68×10^{-3}
0.10	11.91	3.95 ± 0.58	4.95	3422 ± 196	0.791 ± 0.022	4.38×10^{-3}
0.20 (ionic strength 0.2 M)	12.08	8.69 ± 0.41	9.27	4590 ± 75	0.653 ± 0.008	1.30×10^{-3}
0.20 (ionic strength 1.0 M)	12.21	10.2 ± 0.21	9.27	6245 ± 43	0.578 ± 0.004	9.26×10^{-4}
0.40	12.43	17.7 ± 0.68	17.90	7221 ± 104	0.425 ± 0.011	1.72×10^{-3}
0.50	12.51	21.4 ± 0.82	22.20	8353 ± 124	0.382 ± 0.013	2.47×10^{-3}
1.00	12.71	44.4 ± 0.50	43.80	8466 ± 44	0.294 ± 0.003	6.80×10^{-4}

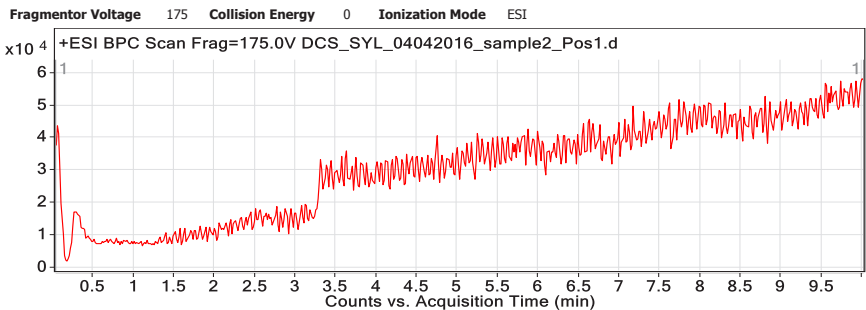
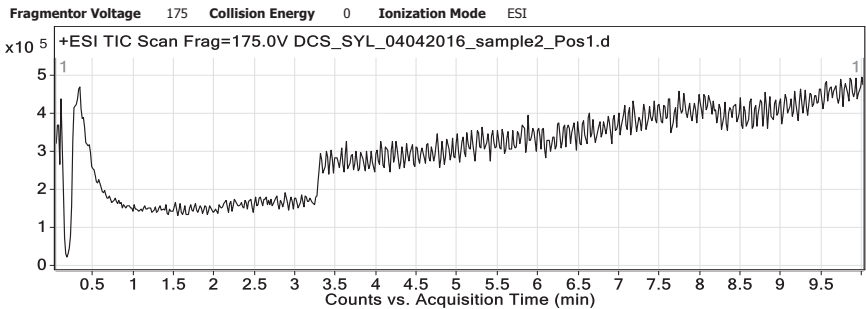
^a Reaction conditions for alkaline hydrolysis of AMPNa₂^b pH was taken after all the ingredients were added except substrate at temperature 60°C^c Residual error of calculated data points to the observed data points.^d Error limits are standard deviations.**Table S2:** consisting of [HCl], pH, and the kinetic parameters (k_{obs} , E_{app} , A_{∞} and $\sum di^2$) for acidic hydrolysis of 0.0001 M AMPNa₂ at 60°C.

[HCl]	pH ^b	$10^7 k_{\text{obs}}/\text{s}^{-1}$	$10^7 k_{\text{calc}}/\text{s}^{-1}$	$E_{\text{app}}/\text{M}^{-1}\text{cm}^{-1}$	A_0	$\sum di^2$ ^c
0.01	1.83	$1.32 \pm 0.06d$	0.27	$4500 \pm 77 d$	$0.744 \pm 0.005 d$	2.27×10^{-3}
0.04	1.38	0.32 ± 0.07	0.75	10004 ± 141	0.468 ± 0.016	7.48×10^{-4}
0.40	0.51	5.52 ± 0.58	6.57	3687 ± 164	0.764 ± 0.010	3.08×10^{-3}
1.00	0.30	16.7 ± 1.00	16.3	3688 ± 91	0.757 ± 0.009	3.36×10^{-3}

^a Reaction conditions for acidic hydrolysis of AMPNa₂^b pH was taken after all ingredients were added except substrate at temperature 60 °C^c Residual error of calculated data points to the observed data points.^d Error limits are standard deviations.

Qualitative Analysis Report

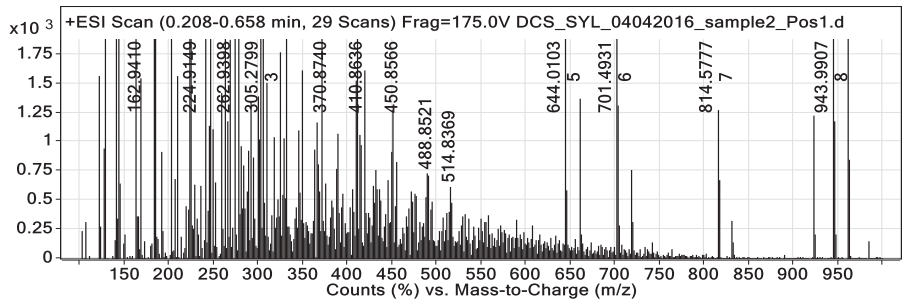
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Sample Type	Sample	Position	Vial 1
Instrument Name	Instrument 1	User Name	
Acq Method	100pg_res_ms(DIRECT RUN).m	Acquired Time	4/4/2016 12:36:04 PM
IRM Calibration Status	All Ions Missed	DA Method	Default.m
Comment			
User Chromatograms			



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

Qualitative Analysis Report



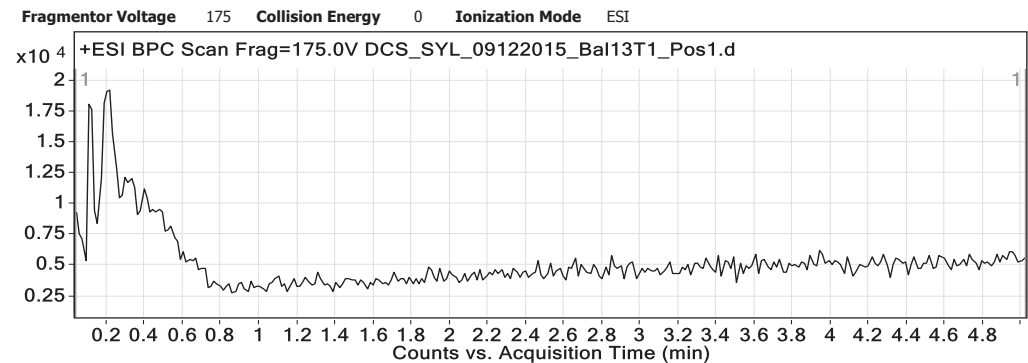
Peak List

m/z	z	Abund
128.9549		5826.8
140.9604		8347.1
142.9658		4483.4
162.941		8360.2
184.9226		4722.7
224.9149		5070.4
262.9398		5207.2
644.0103	1	3589.1
943.9907	1	5302.2
959.9645	1	3657

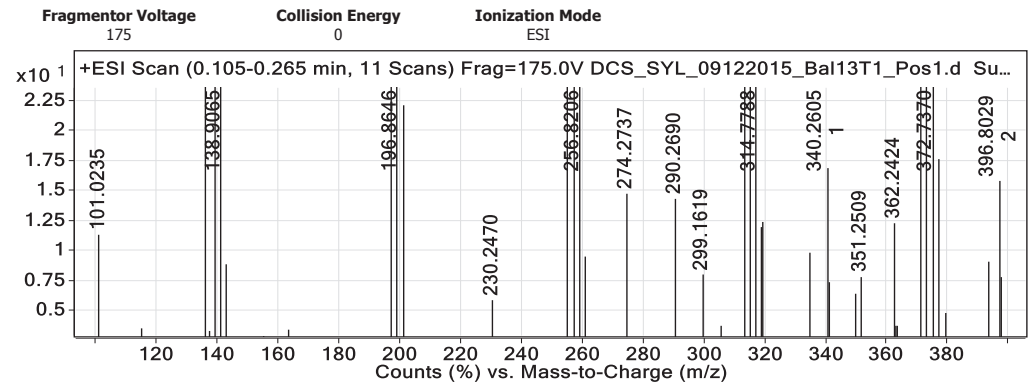
Figure S1: LCMS Spectrum of the alkaline hydrolysis products of AMPNa-2 in 1.0 M NaOH.

Qualitative Analysis Report

Data Filename	DCS_SYL_09122015_Bal13T1_Pos1.d	Sample Name	Bal13T1
Sample Type	Sample	Position	Vial 1
Instrument Name	Instrument 1	User Name	
Acq Method	100pg_res_ms(DIRECT RUN).m	Acquired Time	12/9/2015 1:51:47 PM
IRM Calibration Status	All Ions Missed	DA Method	Default.m
Comment			
User Chromatograms			



User Spectra



Peak List

m/z	Abund
136.0622	6164.7
138.9065	12812.5
140.9034	8241.9
196.8646	9979.2
198.8619	9835
254.8235	11171.9
256.8206	13706.8
258.8174	6775.5
314.7788	8206
372.737	7194.4

Figure S2: Spectrum of the acidic hydrolysis products of AMPNa-2 in 1.0 M HCl.

Table S3: consisting of [TRIS], [glycine], pH, and the kinetic parameters (k_{obs} , E_{app} , A_{∞} and $\sum di^2$) for hydrolysis of 0.0001M AMPNa₂ at 60°C_a.

[glycine] in the form of free acid	pH <i>b</i>	$10^8 k_{\text{obs}}/\text{s}^{-1}$	$E_{\text{app}}/\text{M}^{-1}\text{cm}^{-1}$	A_{∞}	$\sum di^2$ <i>c</i>
20% fa	1.82	42.1 ± 22.9 <i>d</i>	1533 ± 474 <i>d</i>	0.850 ± 0.051 <i>d</i>	2.89×10^{-4}
40% fa	2.00	72.5 ± 22.5	928 ± 123	0.936 ± 0.014	2.56×10^{-4}
[TRIS] in form of free base	pH <i>b</i>	$10^8 k_{\text{obs}}/\text{s}^{-1}$	$E_{\text{app}}/\text{M}^{-1}\text{cm}^{-1}$	A_0	$\sum di^2$ <i>c</i>
80% fb	8.03	9.00 ± 4.16 <i>d</i>	2335 ± 743 <i>d</i>	1.087 ± 0.004 <i>d</i>	3.15×10^{-4}
90% fb	8.42	4.94 ± 1.08	2228 ± 194	1.093 ± 0.008	2.47×10^{-3}

^a Reaction conditions for buffer hydrolysis of AMPNa₂^b pH was taken after all ingredients were added except substrate at temperature 60 °C^c Residual error of calculated data points to the observed data points.^d Error limits are standard deviations.