Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary Information

Synthesis and evaluation of 2-ethynyl-adenosine-5'-triphosphate as a chemical reporter for protein AMPylation

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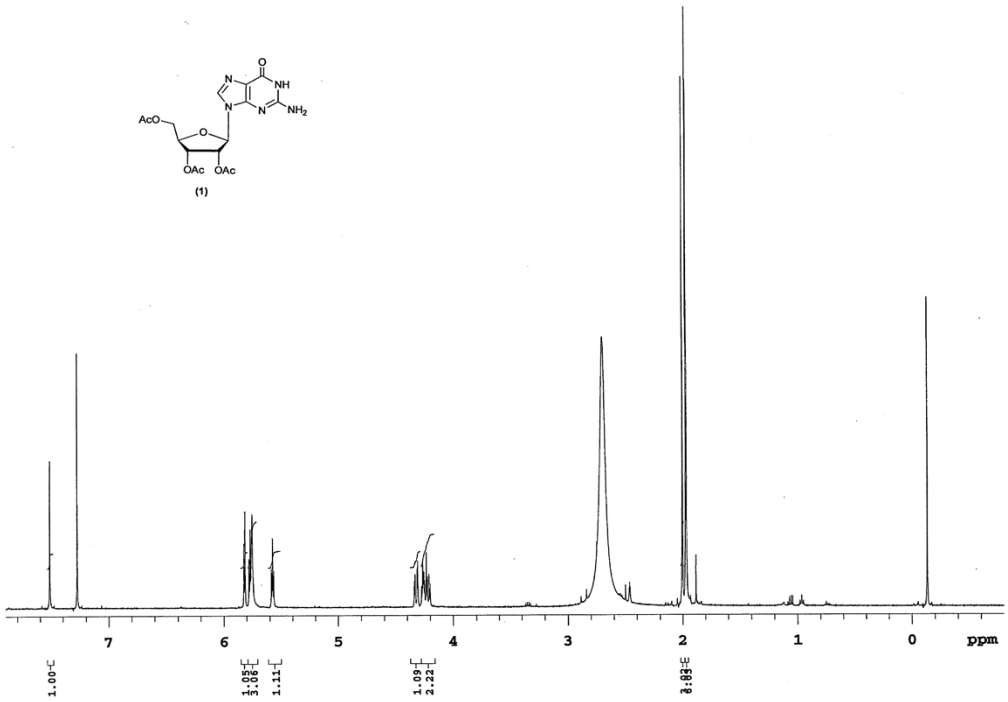

Fig. S1 ^{1}H NMR of 2',3',5'-triacetylguanosine (**1**).

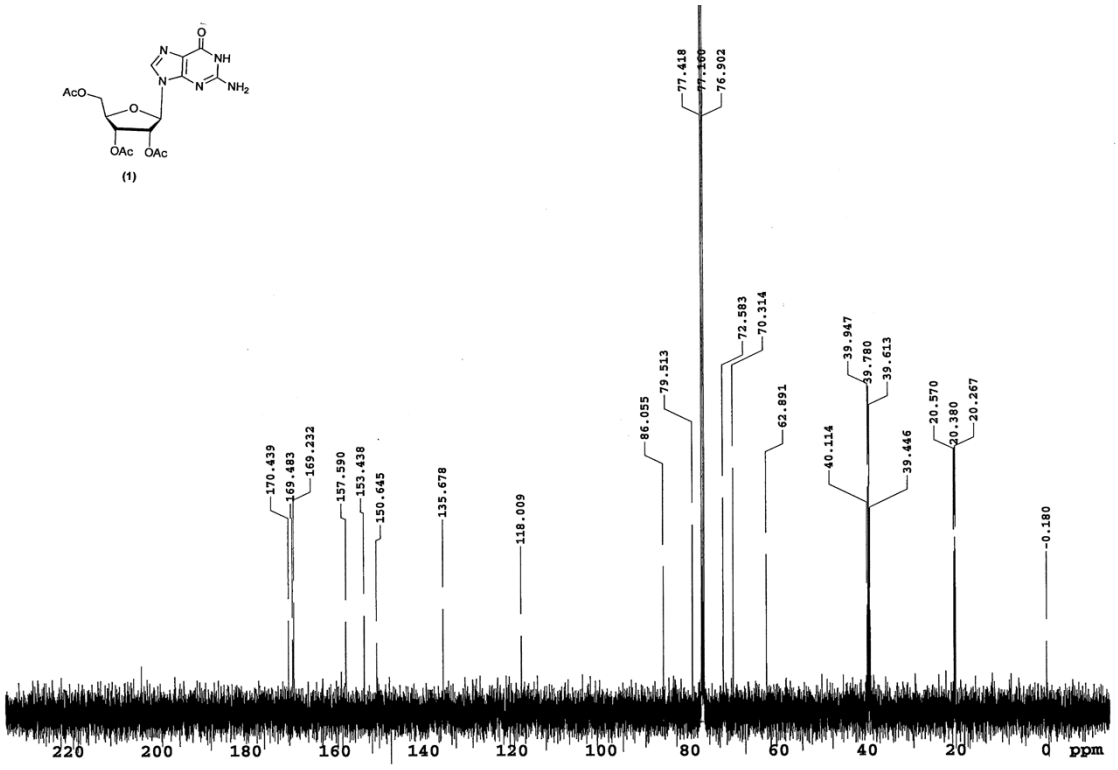

Fig. S2 ^{13}C NMR of 2',3',5'-triacetylguanosine (**1**).

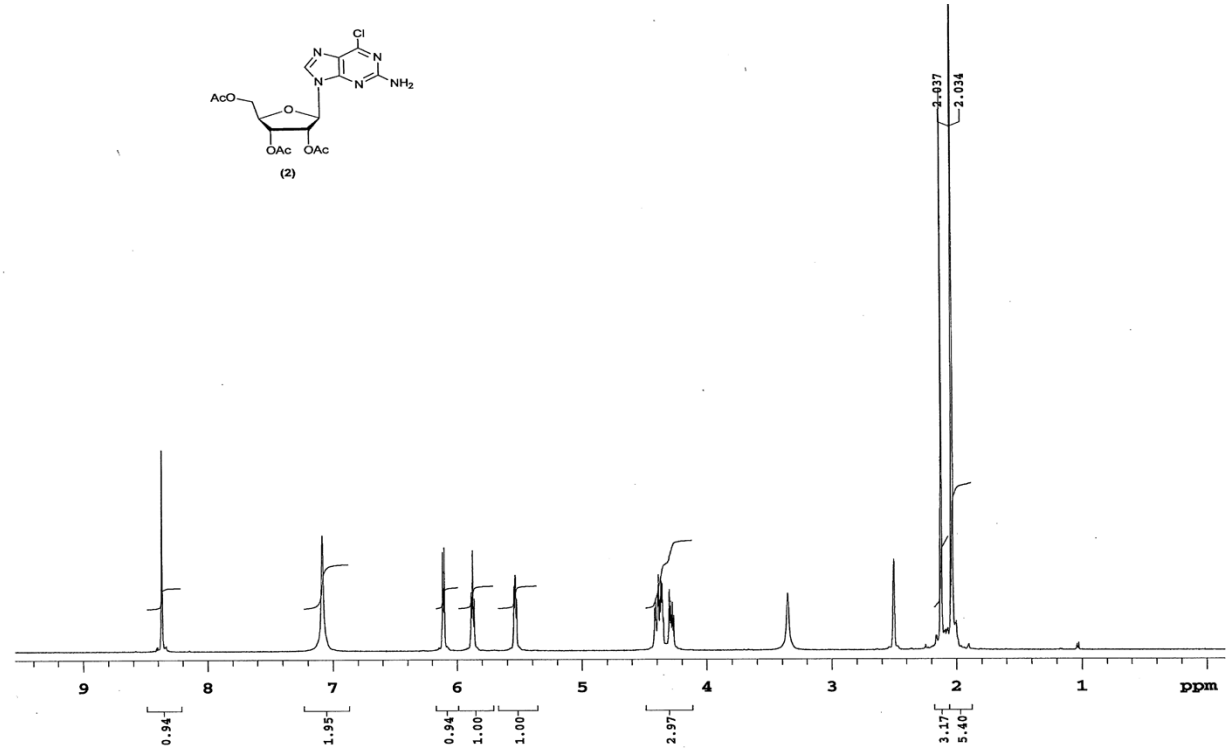

Fig. S3 ^{1}H NMR of 2-amino-6-chloro-9-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)purine (**2**).

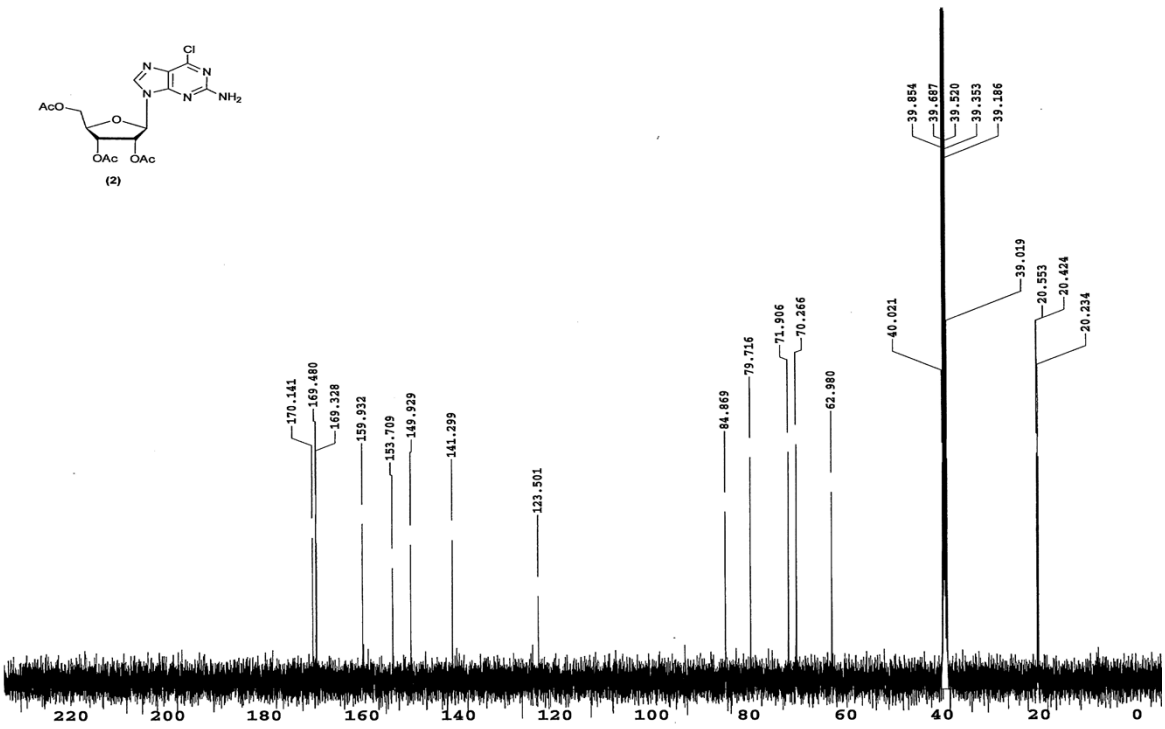

Figure S4. ^{13}C NMR of 2-amino-6-chloro-9-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)purine (**2**).

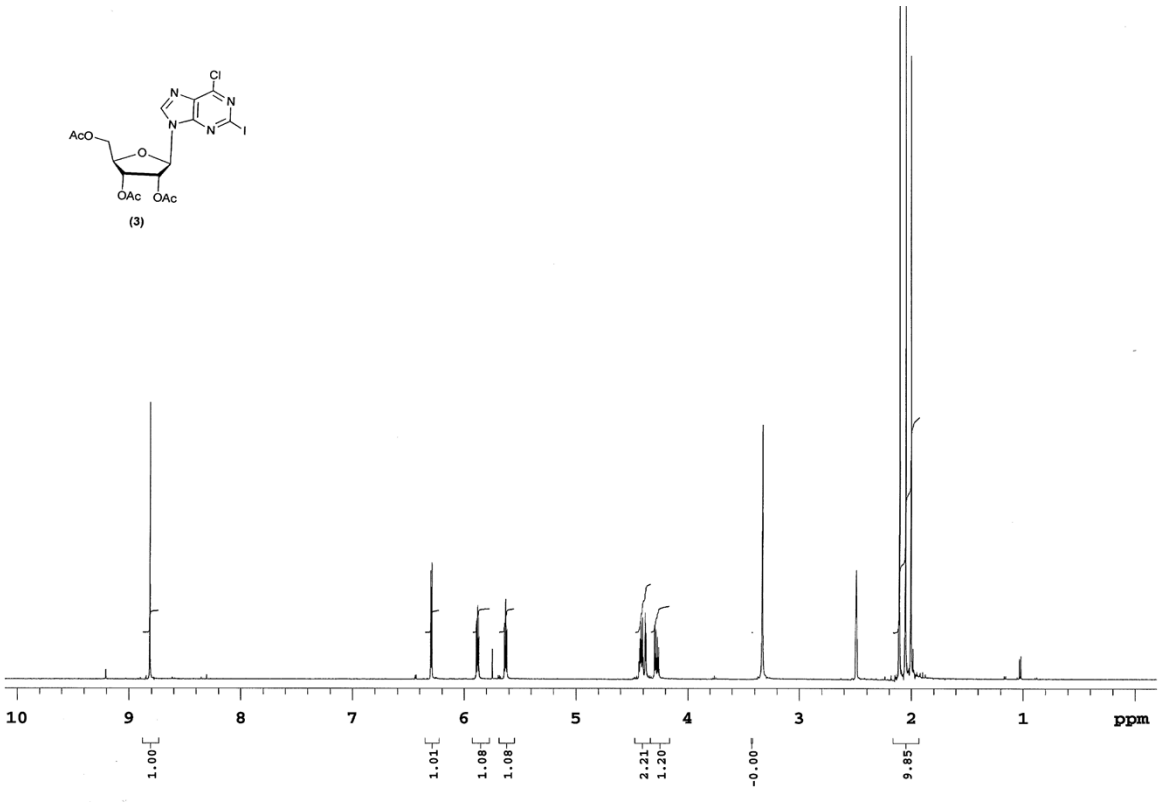

Fig. S5 ^{1}H NMR of 6-chloro-2-iodo-9-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-9H-purine (**3**).

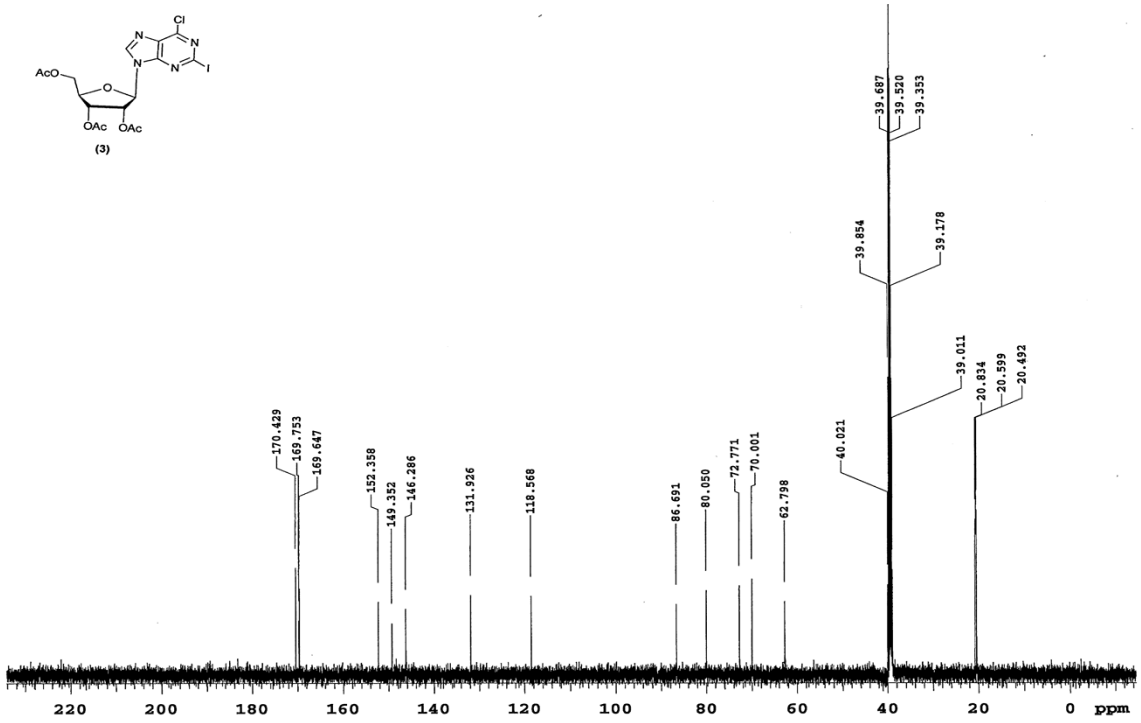

Fig. S6 ^{13}C NMR of 6-chloro-2-iodo-9-(2,3,5-tri-O-acetyl-β-D-ribofuranosyl)-9H-purine (**3**).

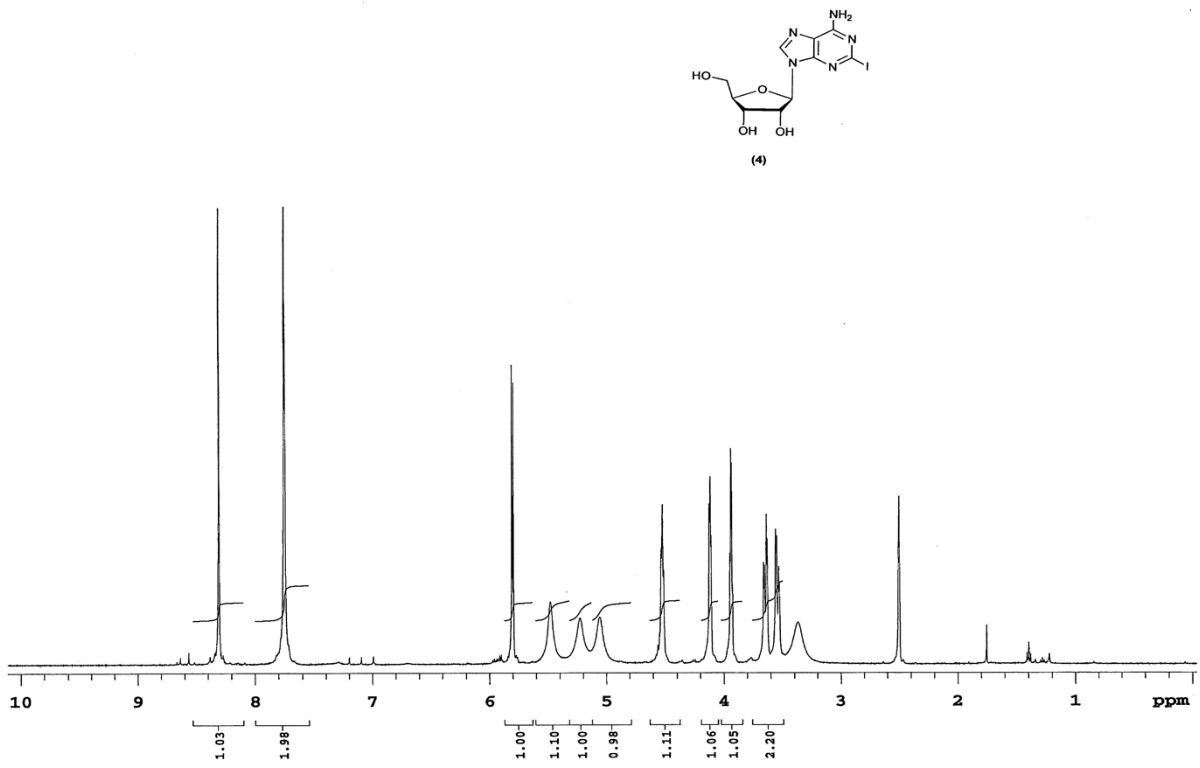

Fig. S7 ^{1}H NMR of 2-iodoadenosine (**4**).

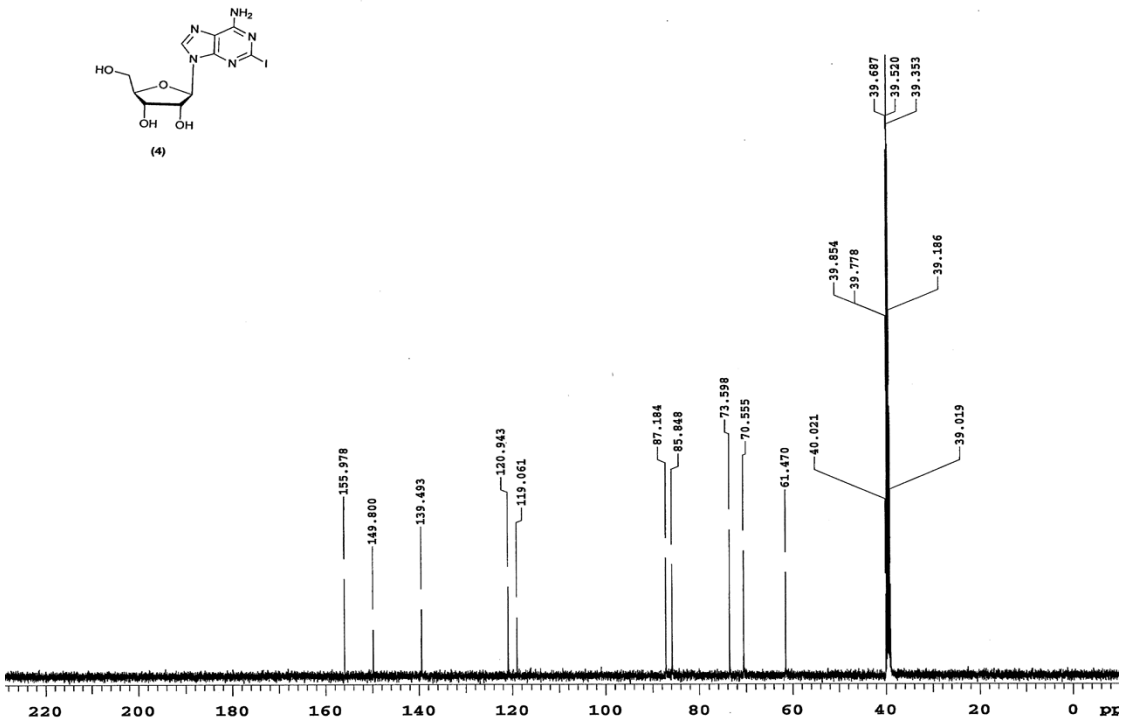

Fig. S8 ^{13}C NMR of 2-iodoadenosine (**4**).

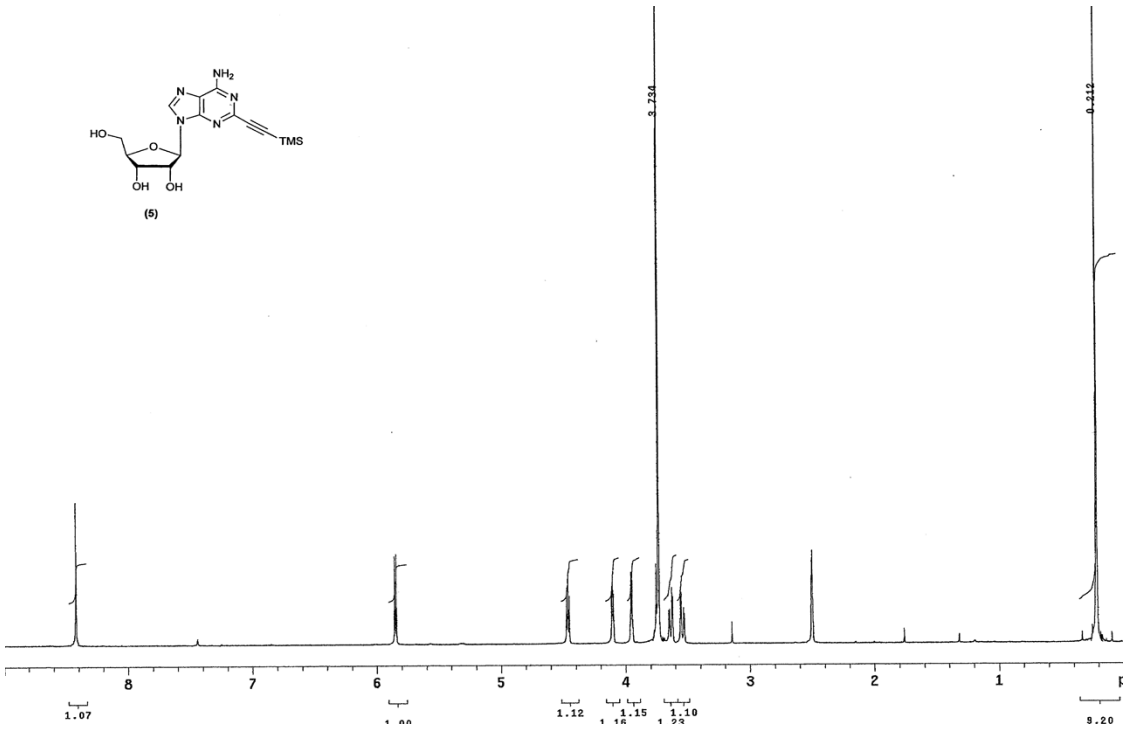

Fig. S9 ^{1}H NMR of 2-[2-(trimethylsilyl)ethynyl]-adenosine (**5**).

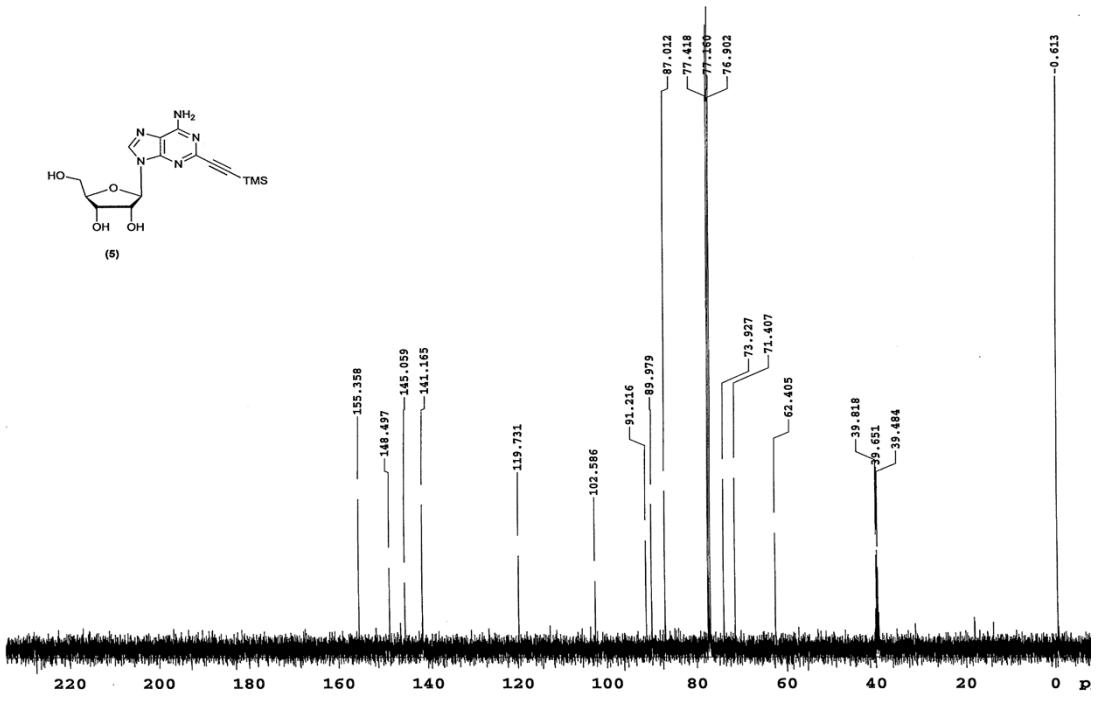

Fig. S10 ^{13}C NMR of 2-[2-(trimethylsilyl)ethynyl]-adenosine (**5**).

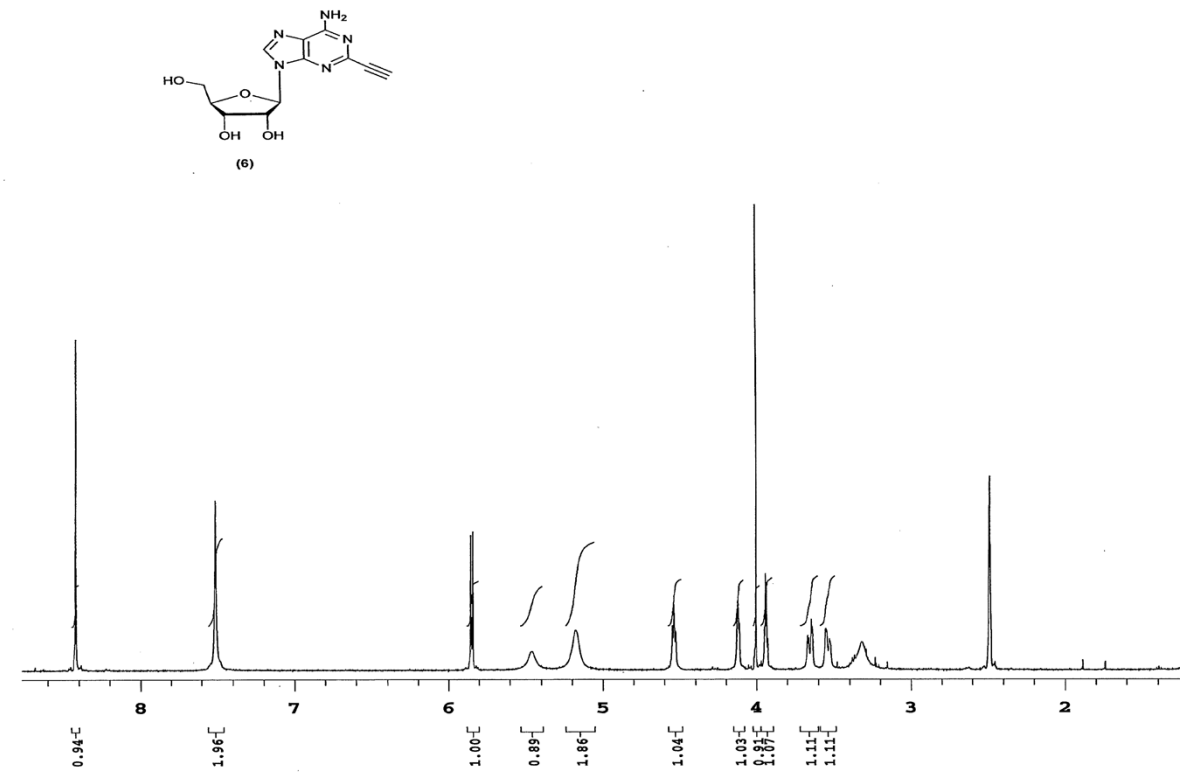

Fig. S11 ^{1}H NMR of 2-ethynyladenosine (**6**).

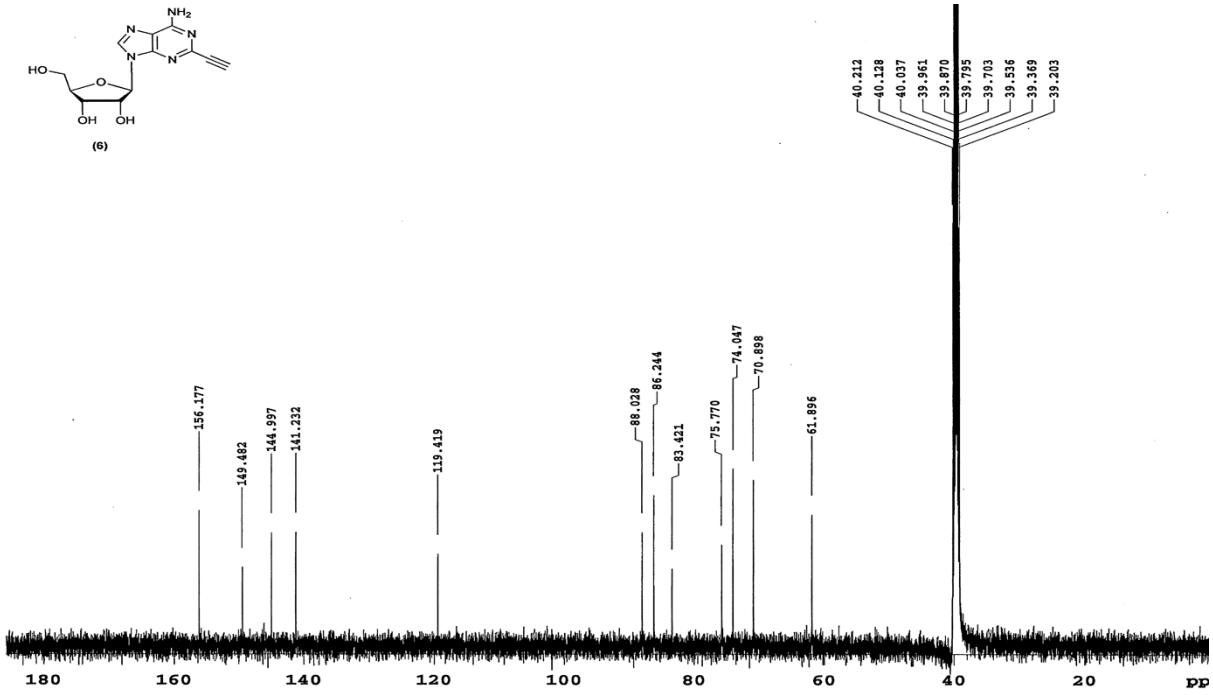

Fig. S12 ^{13}C NMR of 2-ethynyladenosine (**6**).

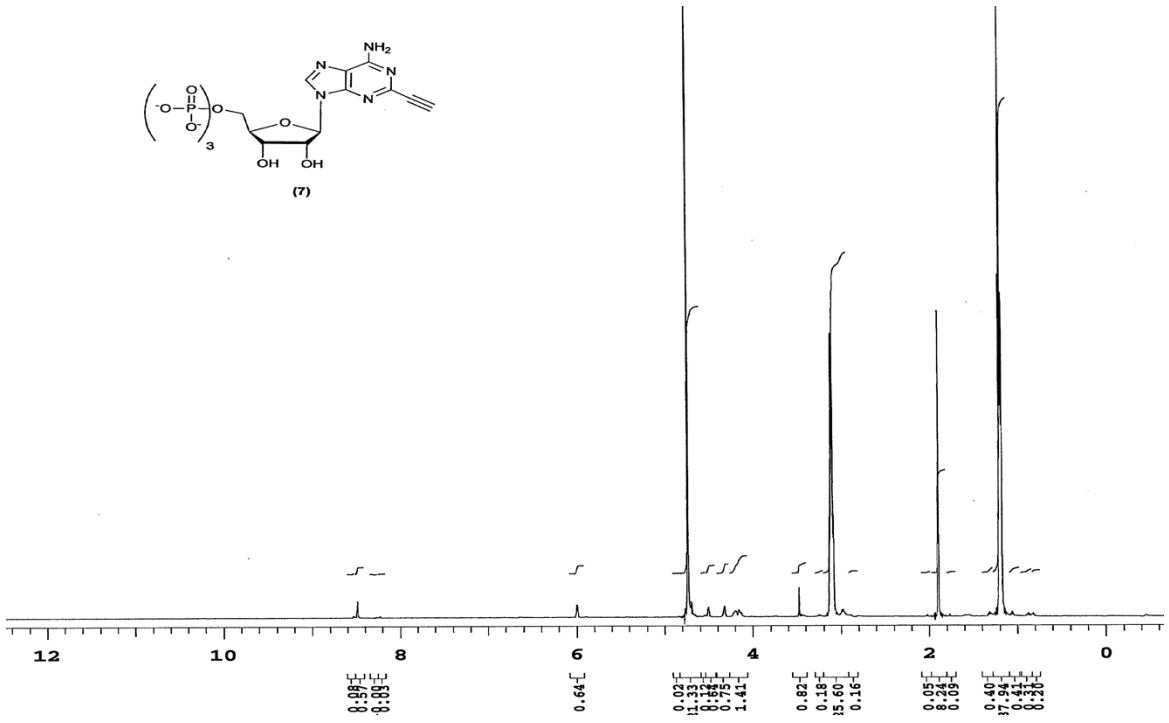

Fig. S13 ^{1}H NMR of 2-ethynyl-adenosine-5'-triphosphate (2eATP)(**7**) in triethylammoniumacetate buffered D_2O.

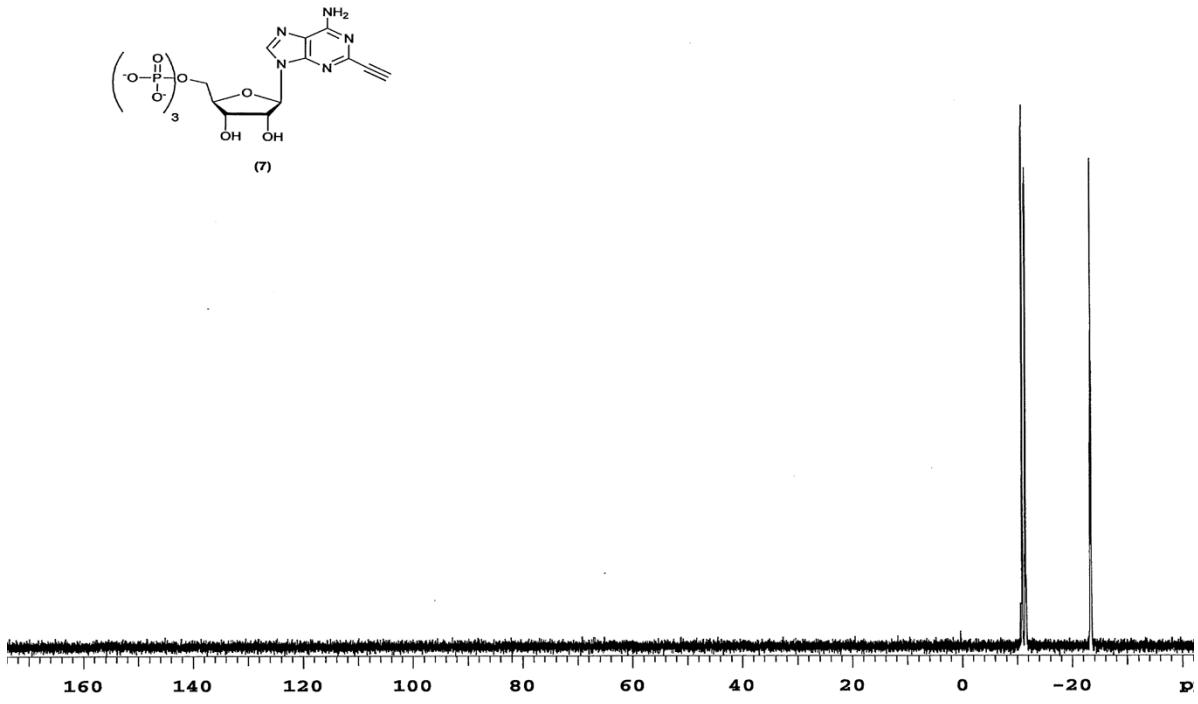

Fig. S14 ^{31}P NMR of 2-ethynyl-adenosine-5'-triphosphate (2eATP)(**7**).

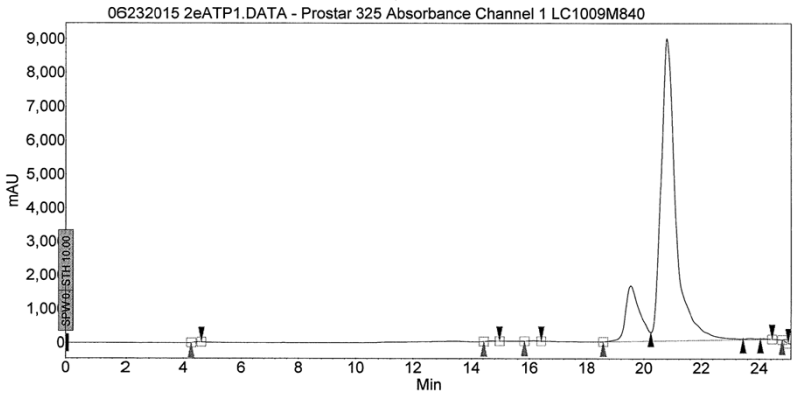

Fig. S15 HPLC chromatogram of 2eATP reaction separation.

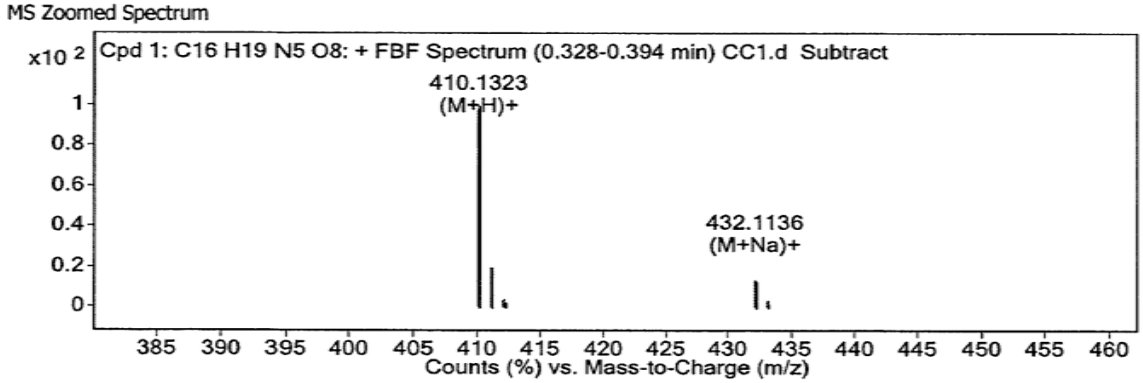

Fig. S16 Mass spectrum of compound **1** (calculated mass: 410.1312).

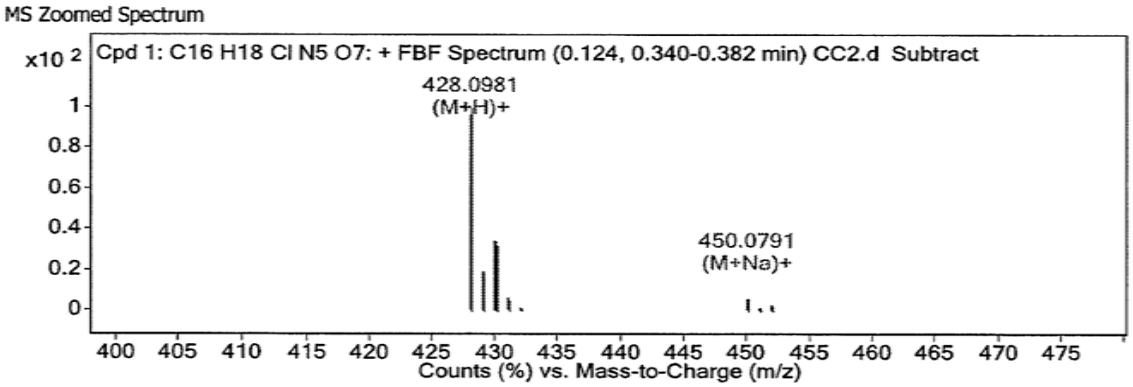

Fig. S17 Mass spectrum of compound **2** (calculated mass: 428.0973).

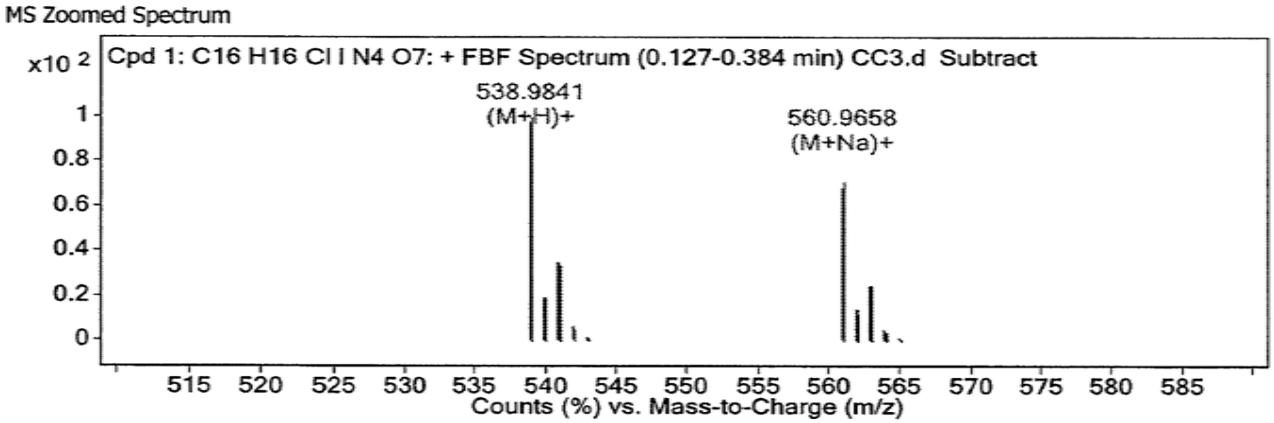

Fig. S18 Mass spectrum of compound 3 (calculated mass: 538.9831).

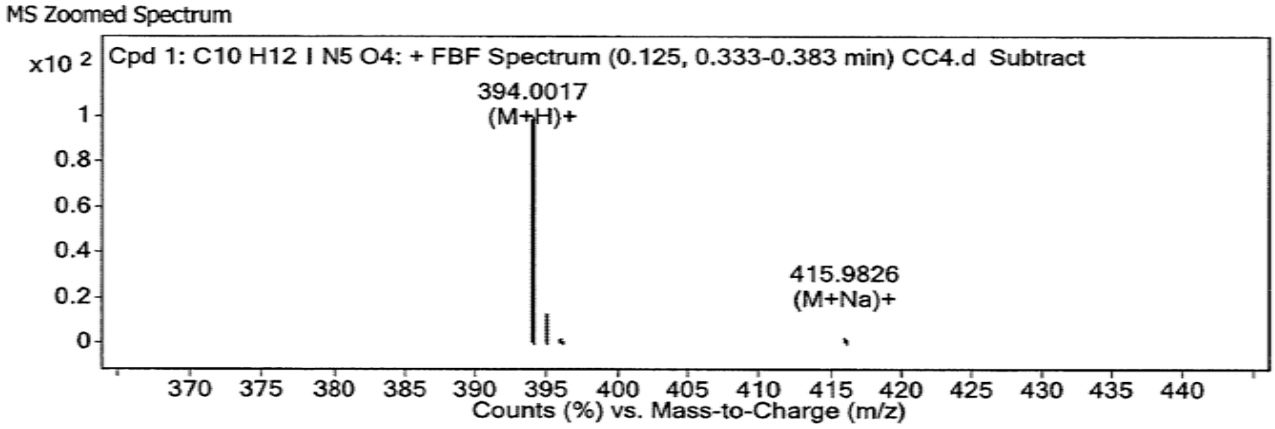

Fig. S19 Mass spectrum of compound 4 (calculated mass: 394.0012).

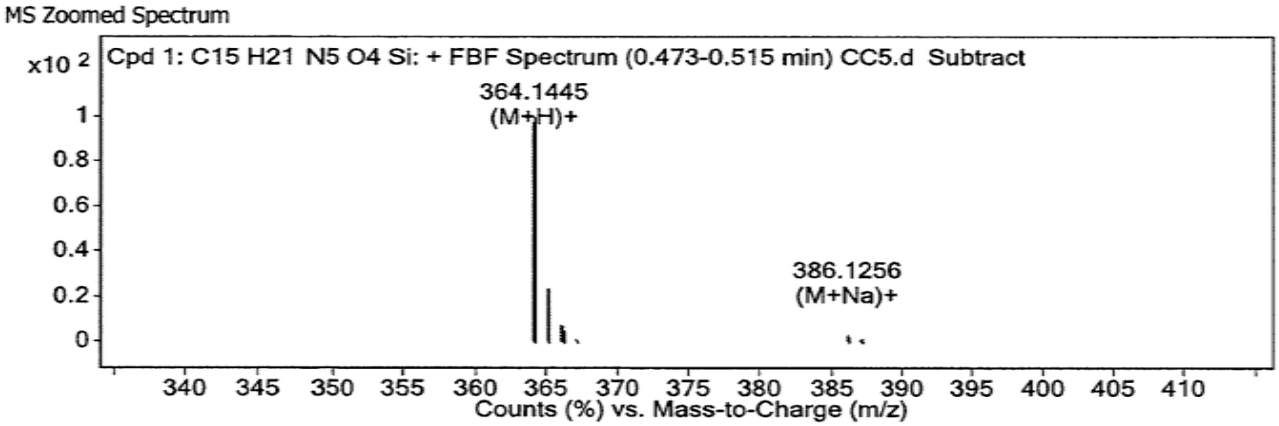

Fig. S20 Mass spectrum of compound 5 (calculated mass: 364.1441).

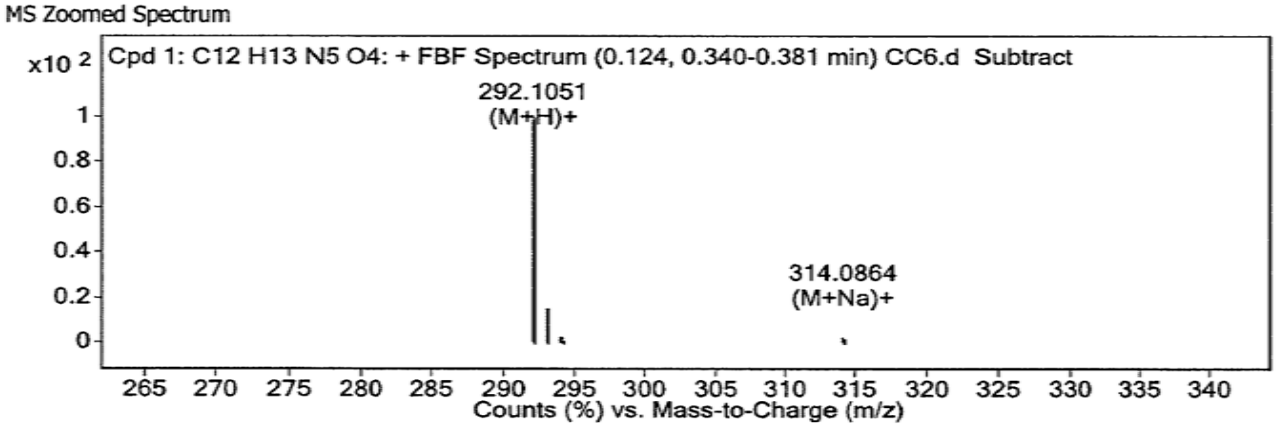

Fig. S21 Mass spectrum of compound 6 (calculated mass: 292.1046).

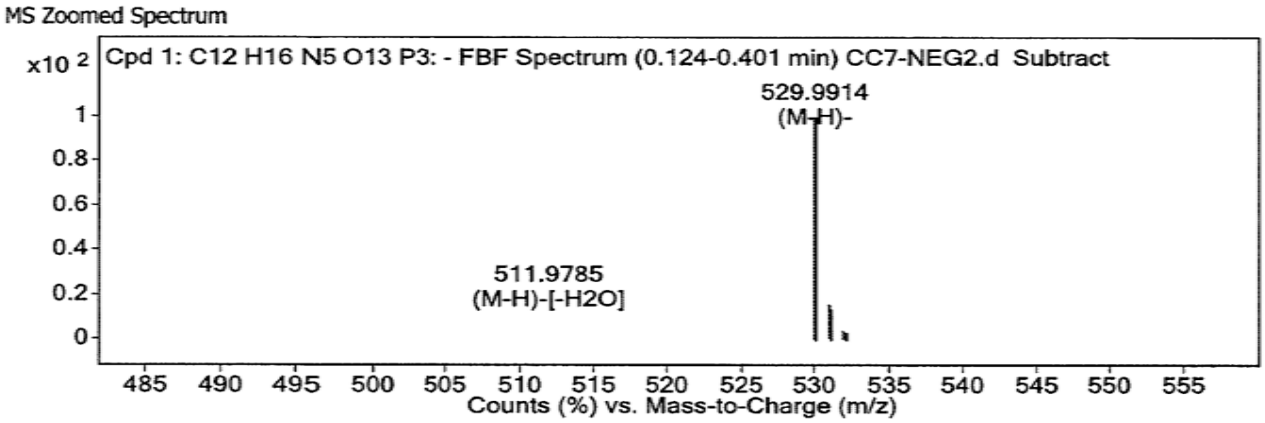

Fig. S22 Mass spectrum of compound 7 (calculated mass: 529.9879).

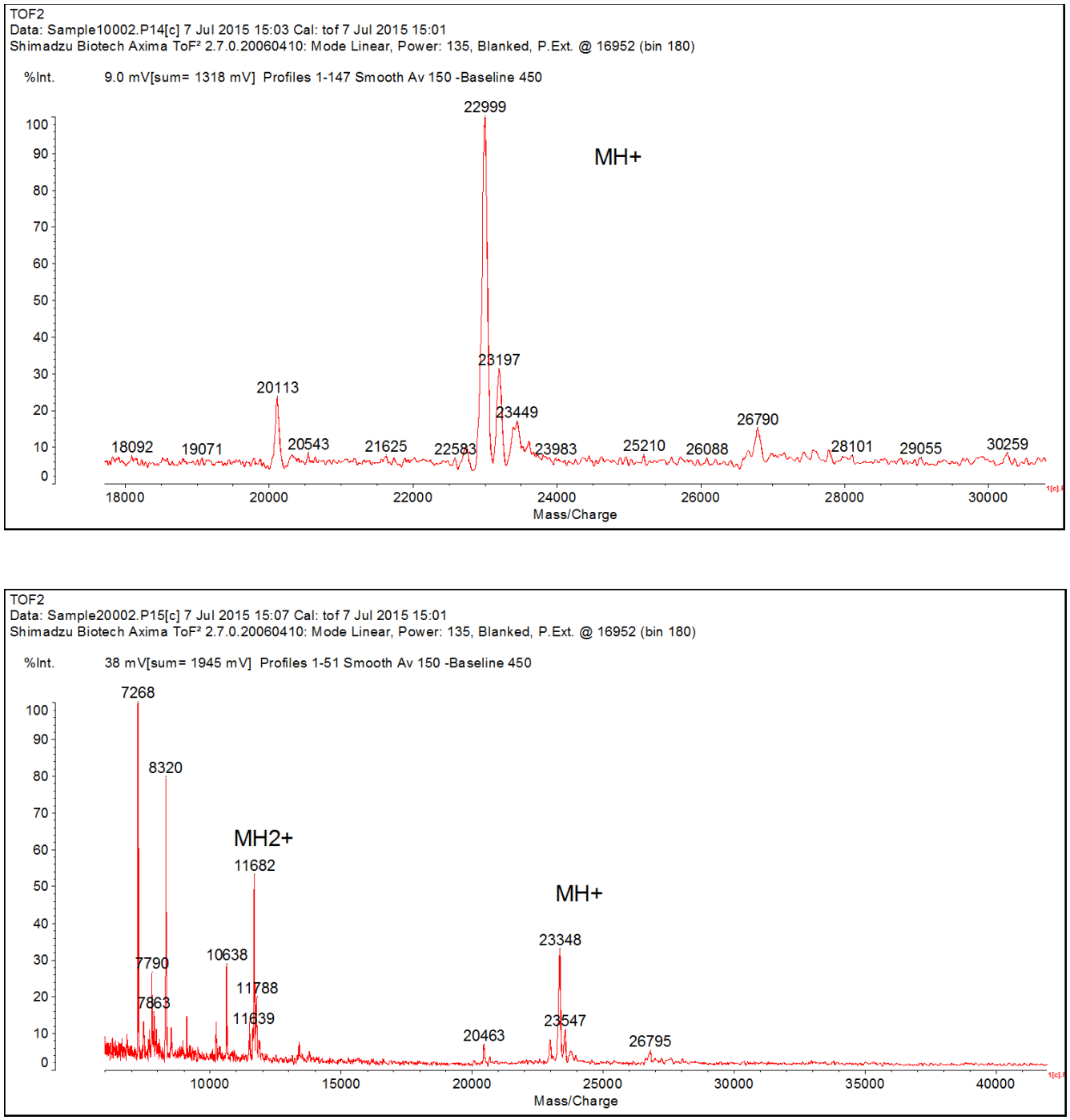

Fig. S23 The modification of Cdc42 with 2eAMP was confirmed by MALDI mass spec. The top spectrum is Cdc42 that was incubated with VopS in the absence of 2eATP. The bottom spectrum shows Cdc42 that was incubated with VopS in the presence of 2eATP. The expected mass difference is 353 Da for the addition of the 2eAMP group.