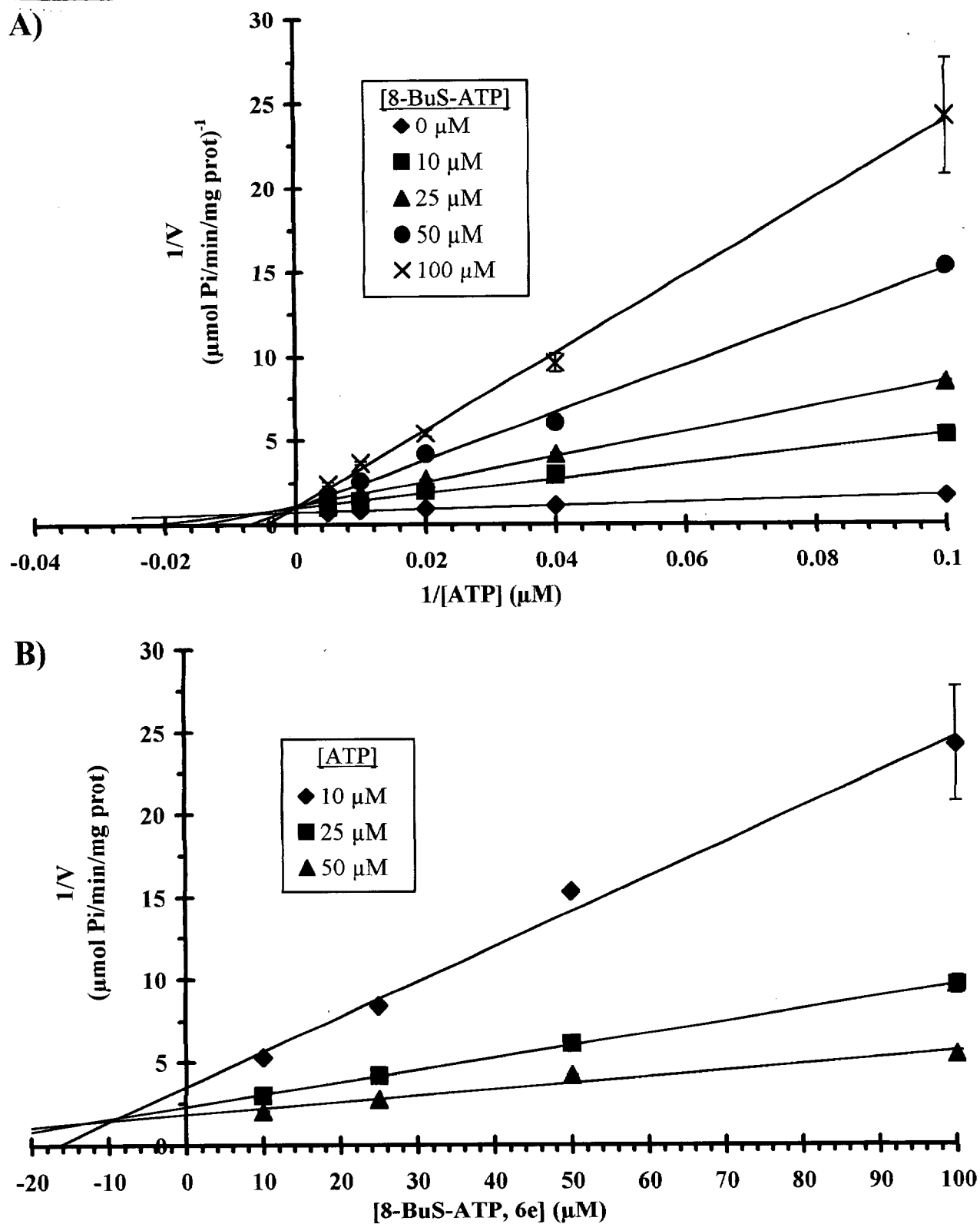
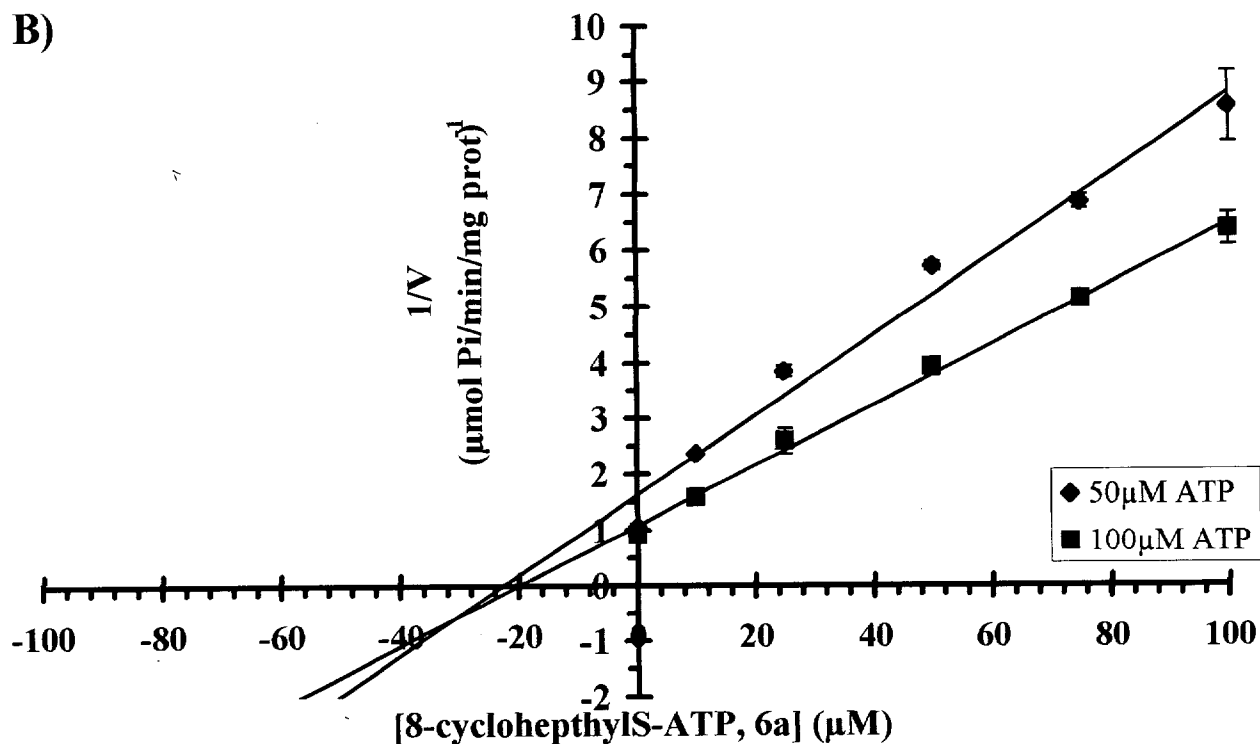
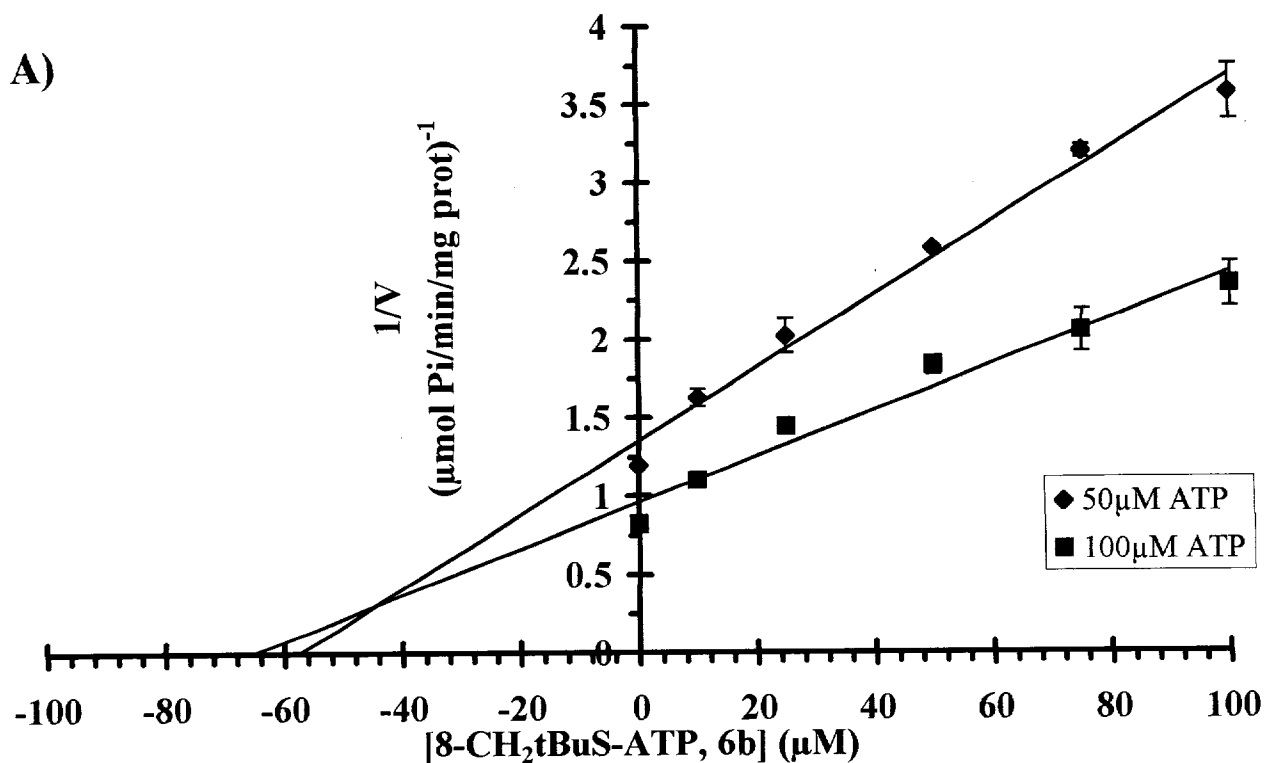


Figure S1. Inhibitory effect of 8-BuS-ATP, 6e, on ATP hydrolysis by NTPDase.



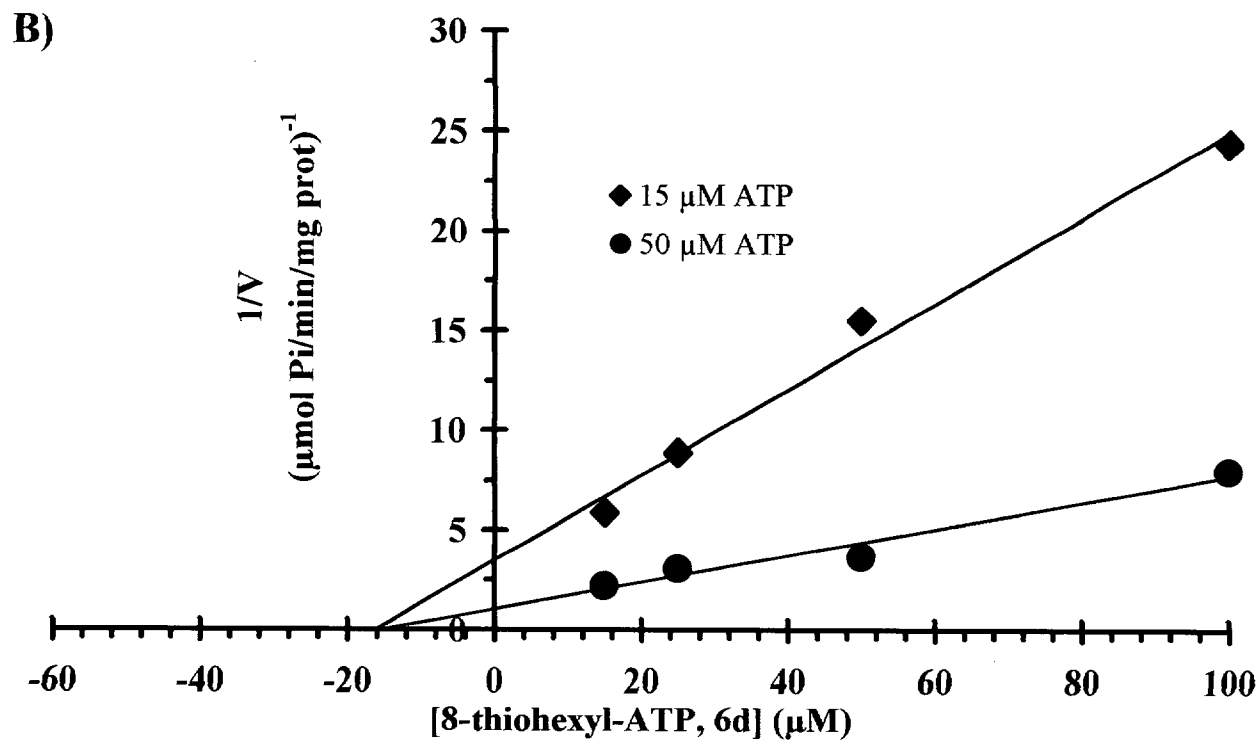
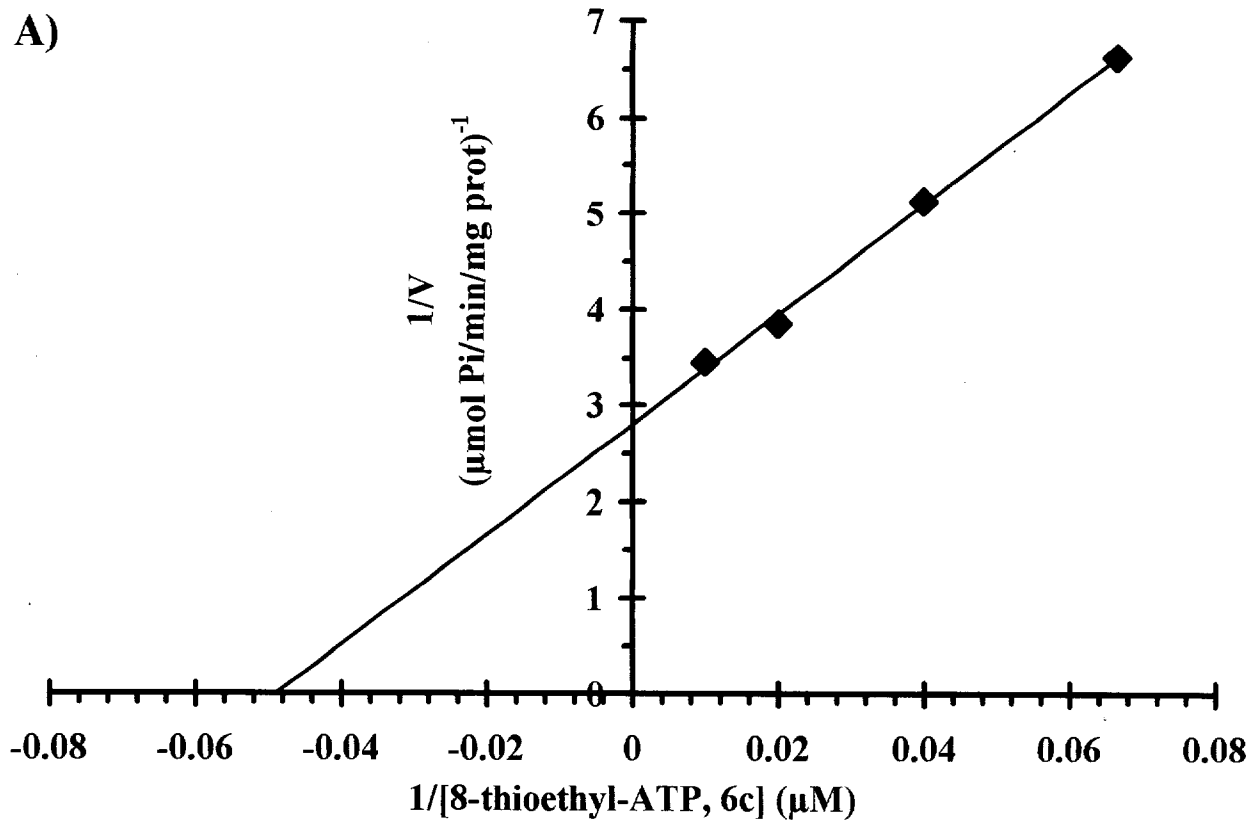
8-BuS-ATP produce a competitive inhibition with an estimated K_i of 10 μM . Results are expressed as the mean \pm SEM of two experiments each in duplicate.

Figure S2. Dixon representations of 8-CH₂tBuS-ATP, 6b, (A) and 8-cycloheptylS-ATP, 6a, (B) inhibition.



Both analogues act as mixed type inhibitors with estimated K_i of 45 and 31 μM for 8-tBuCH₂ ATP, 6b, and 8-cycloheptylS-ATP, 6a, respectively. Experiments were carried out in triplicate and expressed as the mean \pm SEM.

Figure S3. A) Hydrolysis of 8-thioethyl-ATP, 6c, by NTPDase. B) Dixon representation of 8-thiohexyl, 6d, inhibition.



Analogue **6d** act as a non-competitive inhibitor with an estimated K_i of 16 μM . Experiments was carried out in triplicate and expressed as the mean \pm SEM.