Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Development of a selective and highly sensitive fluorescence assay for nucleoside triphosphate diphosphohydrolase1 (NTPDase1, CD39)

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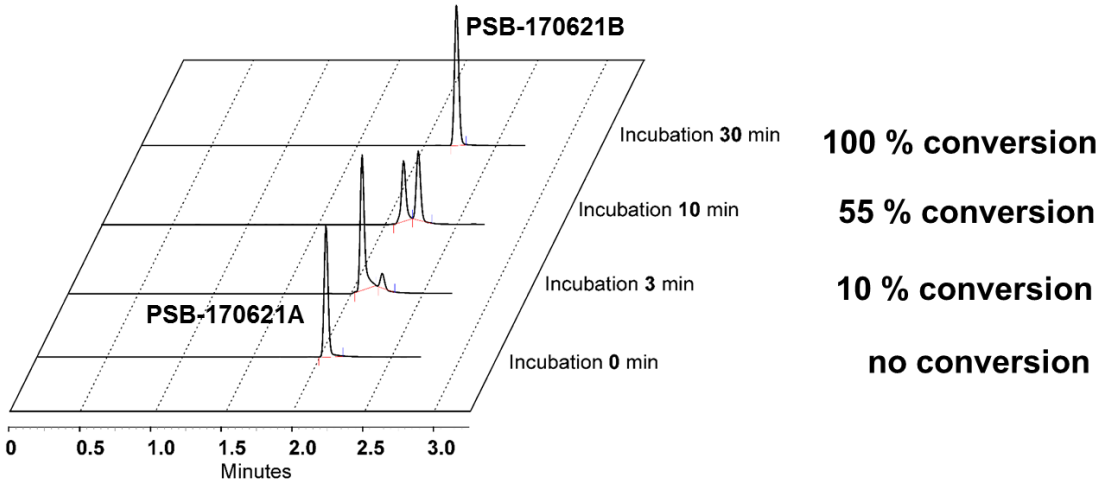

Fig. S1. CE chromatograms with different incubation times for the hydrolysis of PSB-170621A to its enzyme product PSB-170621B. The separation conditions for the reverse operation were: 50 mM phosphate buffer (pH 6.5), effective capillary length of 10 cm x 50 µm (id), electrokinetic injection (6 kV, 30 s), separation at 15 kV and detection at 488 nm (excitation) and 520 nm (emission). The samples were diluted 100-fold with reaction buffer before CE measurements.

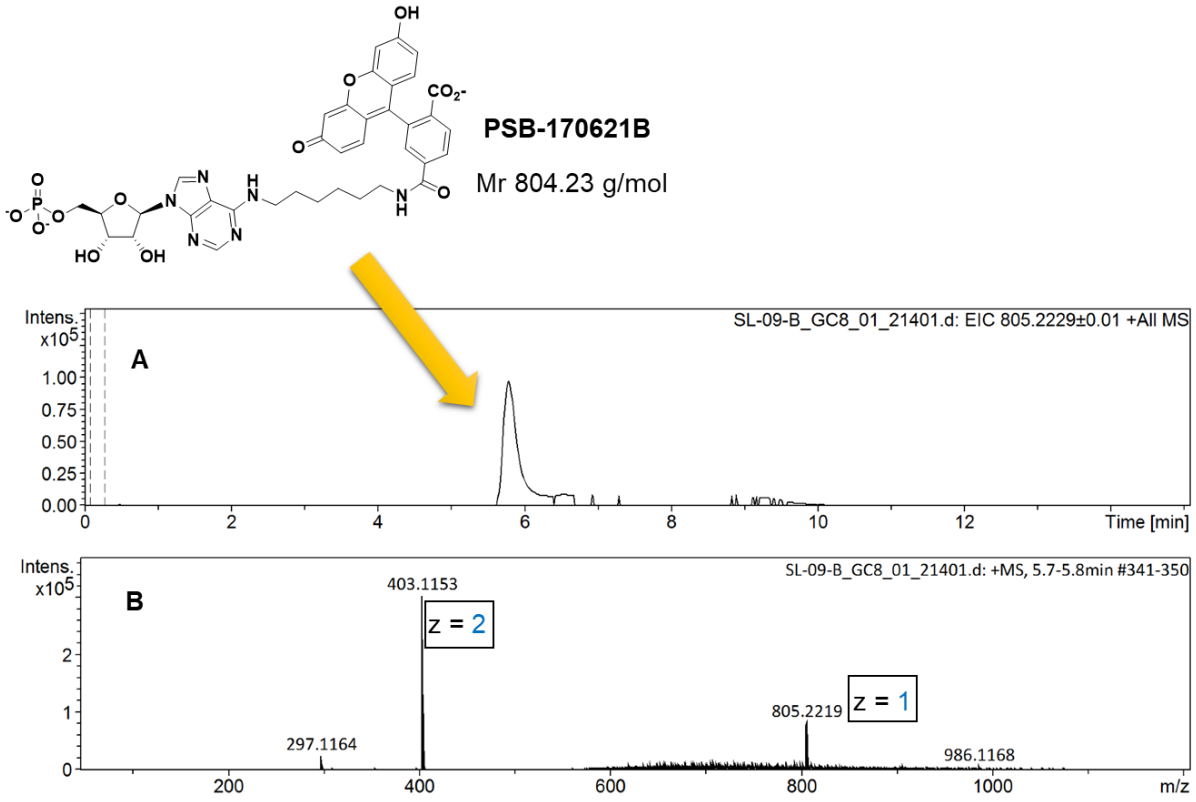

Fig. S2. LC-MS chromatogram of PSB-170621B. (**A**) Only one peak with a retention time of 5.8 min was observed in the UV/VIS chromatogram, (**B**) Two M/z values were obtained for the single peak in the UV/VIS chromatogram (M/z 805,2219 with z = 1 and M/z 403,1153 with z = 2).

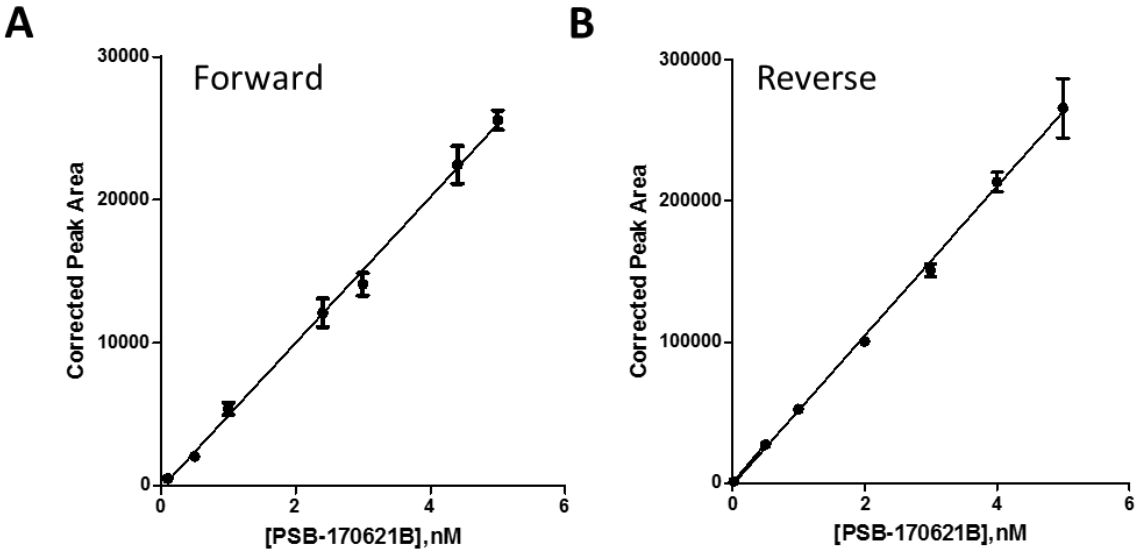

Fig. S3. Calibration curves for the forward operation (**A**) and the reverse operation (**B**).

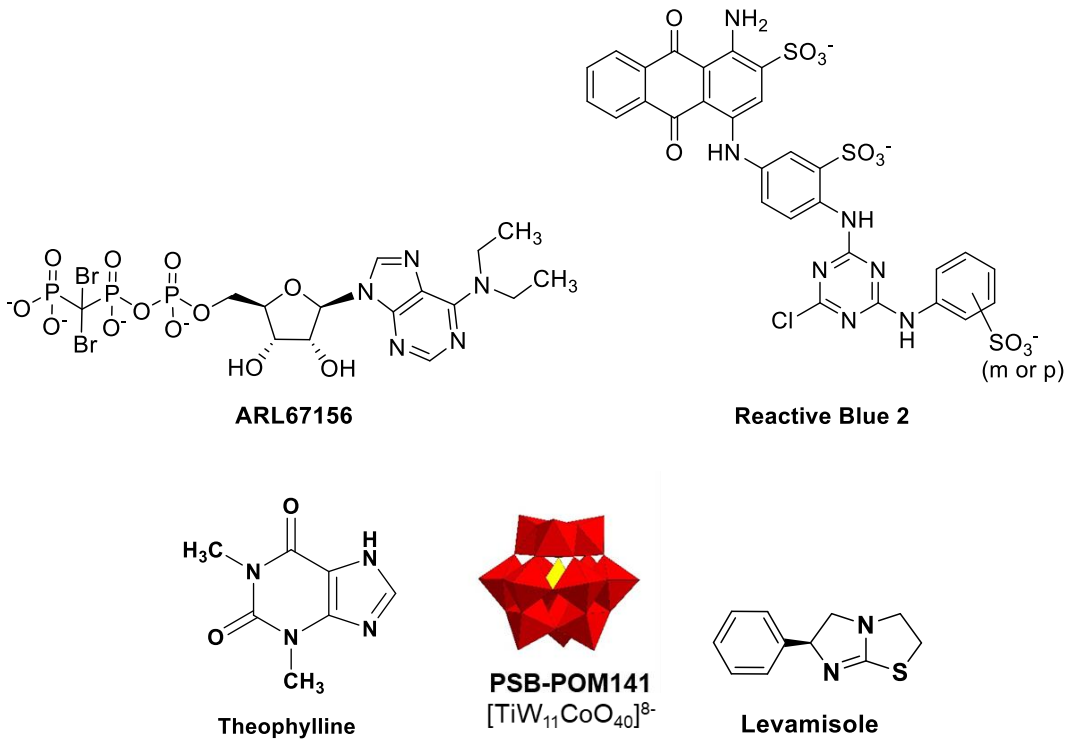

Fig. S4. Structural formulae of the investigated inhibitors.

Table S1. Kinetic data of PSB-170621A at different ectonucleotidases

	NTPDases				NPPs		APs
	NTPDase1	NTPDase2	NTPDase3	NTPDase8	NPP1	NPP3	TNAP
K_m (µM)	19.6	55.5	13.3	105	37.5	47.6	12.5
k_{cat} (10^{-3} x s^{-1})	119	4.94	22.5	38.7	1.99	1.05	24.8
k_{cat}/K_m (M^{-1} x s^{-1})	6070	89.0	1690	369	53.1	22.1	1980