Supplementary data:

Structures of *Burkholderia thailandensis* nucleoside kinase: implications for the catalytic mechanism and nucleoside selectivity

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Supplementary figure legends

Supplementary Figure 1

Sequence alignment between BthNK, MtADK, MjNK, and human ADK (hADK). The residue number for hADK is based on the numbering reported in the PDB file (PDB code, 1BX4). The conserved "*NXXE*" motif crucial for Mg^{2+} binding is boxed. The conserved residues for the binding of the ribose moiety of the nucleoside are highlighted in yellow. The diversified residues for the binding of the base moiety of nucleoside are highlighted in light pink. The Phe residue for the stacking interaction with the base moiety of the bound nucleoside is also highlighted in orange. Identical, strongly similar, and weakly similar residues are in red, green, and light blue, respectively.

Supplementary Movie 1

Conformational dynamics of BthNK between asymmetric open, semiclosed and closed form. In the semiclosed and closed forms, the bound ligands are also shown in stick representation.

Supplementary Movie 2

The same as Supplementary Movie 1 but from a different point of view. The images in this movie were created by an approximate 90° rotation of the images in Supplementary Movie 1.

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BthNK     1 --------------MATLICGSIAYDNIMTFEGRFREHILPDQVHLINLSFLVPTMRREF  46
MtADK     1 --------------MTIAVTGSIATDHLMRFPGRFSEQLLPEHLHKVSLSFLVDDLVMHR  46
MjNK      1 ---------MGGKMEKITCVGHTALDYIF------NVEKFPE---PN-TSIQIPSARKYY  41
hADK      5 ----RENILFGMGNPLLDISAVVDKDFLDKYSLKPNDQILAEDKHKELFDELVKKFKVEY  60


BthNK    47 --GGCAGN----IAYALNLLGGDARMMGTLGA-VDAQPYLDRMDALGLSREYVRVLPDTY  99
MtADK    47 --GGVAGN----MAFAIGVLGGEVALVGAAG--ADFADYRDWLKARGVNCDHVLISETAH  98
MjNK     42 --GGAAAN----TAVGIKKLGVNSELLSCVGYDFKNSGYERYLKNLDINISKLYYSEEEE  95
hADK     61 HAGGSTQNSIKVAQWMIQQPHKAATLFGCIGIDKFGEILKRKAAEAHVDAHYYEQNEQPT 120


BthNK   100 SAQAMITTDLDNNQITAFHPGAMMQS--HVNHAGEAKDIK---------LAIVGPDGFQG 148
MtADK    99 TARFTCTTDVDMAQIASFYPGAMSEAR-NIKLADVVSAIGKP------ELVIIGANDPEA 151
MjNK     96 TPKAWIFTDKDNNQITFFLWGAAKHYK-ELNPPNFNTEIVH---------IATGDPE--- 142
hADK    121 GTCAACITGDNRSLIANLAAANCYKKEKHLDLEKNWMLVEKARVCYIAGFFLTVSPE--S 178


BthNK   149 MVQHTEELAQAGVPFIFDPGQ-GLPLFDGATLRRSIELATYIAVNDYEAKLVCDKTGWSE 207
MtADK   152 MFLHTEECRKLGLAFAADPSQ-QLARLSGEEIRRLVNGAAYLFTNDYEWDLLLSKTGWSE 210
MjNK    143 FNLKCAKKAYGNNLVSFDPGQ-DLPQYSKEMLLEIIEHTNFLFMNKHEFERASNLLNFEI 201
hADK    179 VLKVAHHASENNRIFTLNLSAPFISQFYKESLMKVMPYVDILFGNETEAATFAREQGFET 238


BthNK   208 DEI--------------ASRVQALIITRGEHGATIRHRDG--TEQIPAVRAERVIDPTGC 251
MtADK   211 ADV--------------MAQIDLRVTTLGPKGVDLVEPDGT-TIHVGVVPETSQTDPTGV 255
MjNK    202 DDY--------------LERVDALIVTKGSKGSVIYTKDK--KIEIPCIKAGKVIDPTGA 245
hADK    239 KDIKEIAKKTQALPKMNSKRQRIVIFTQGRDDTIMATESEVTAFAVLDQDQKEIIDTNGA 298


BthNK   252 GDAFRGGLLYGIEHGFDWATAGRLASLMGALKIAHQGPQTYAPTRAEIDARFETAFGYRP 311
MtADK   256 GDAFRAGFLTGRSAGLGLERSAQLGSLVAVLVLESTGTQEWQWDYEAAASRLAGAYGEHA 315
MjNK    246 GDSYRAGFLSAYVKGYDLEKCGLIGAATASFVVEAKGCQTNLPTWDKVVERLEKHRI--- 302
hADK    299 GDAFVGGFLSQLVSDKPLTECIRAGHYAASIIIRRTG---------CTFPEKPDFH----- 345


BthNK   312 K-------- 312
MtADK   316 AAEIVAVLA 324
MjNK        --------
hADK        --------
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Supplementary Fig. 1