1. Phylogeny  
   Cyclin‐dependent kinase 1 (CDK1), also known as CDC2 or CDC28, represents the founding member of the cyclin‐dependent kinase family and is highly conserved across eukaryotes. Orthologs have been identified in yeasts (e.g., Saccharomyces cerevisiae and Schizosaccharomyces pombe) as well as in metazoans including mammals, where CDK1 is indispensable for cell cycle progression. CDK1 is grouped within the serine/threonine protein kinases and forms part of a core evolutionary network of cell‐cycle regulators, showing strong phylogenetic relationships with other CDKs that control distinct phases of the cell cycle (brown2015cdk1structuresreveal pages 1-2, harper2001cyclindependentkinases pages 2-4, malumbres2005mammaliancyclindependentkinases pages 1-2).
2. Reaction Catalyzed  
   CDK1 catalyzes the transfer of the terminal γ‐phosphate group from ATP to the hydroxyl group of a serine or threonine residue in its protein substrates. In chemical terms, its reaction can be described as follows:  
   ATP + [protein]–OH → ADP + [protein]–O–PO3²⁻ + H⁺ (template).
3. Cofactor Requirements  
   The kinase activity of CDK1 requires the presence of divalent metal ions, with Mg²⁺ serving as an essential cofactor for optimal ATP binding and catalytic function. This Mg²⁺ dependency is a typical feature among protein kinases (template, shafiq2011molecularmodellingand pages 21-26).
4. Substrate Specificity  
   CDK1 exhibits substrate specificity primarily toward serine and threonine residues that are immediately followed by a proline, defining a minimal consensus motif of S/T-P. In many cases, additional sequence elements or docking interactions provided by cyclin partners further refine substrate recognition. Thus, substrates generally display proline-directed phosphorylation motifs and, in certain contexts, extended motifs that include basic residues at positions downstream of the phosphorylation site (harper2001cyclindependentkinases pages 2-4, errico2010identificationofsubstrates pages 3-4).
5. Structure  
   CDK1 possesses a classical protein kinase fold with a smaller, β‐sheet–rich N‐terminal lobe and a larger, predominantly α‐helical C‐terminal lobe. A key structural element is the PSTAIRE motif, found in the C-helix, which is critical for cyclin binding and proper positioning of catalytic residues. The activation segment (T-loop) of CDK1 undergoes marked conformational changes upon cyclin association and subsequent phosphorylation, thereby creating a fully active kinase conformation. Although monomeric CDK1 shares an overall fold with CDK2, it displays unique variations in thermal stability, the cyclin interface, and the dynamics of its activation loop that dictate its distinct regulatory properties (brown2015cdk1structuresreveal pages 1-2, malumbres2014cyclindependentkinases pages 3-5, wood2018structuralinsightsinto pages 1-2).
6. Regulation  
   The regulation of CDK1 is multifaceted and chiefly controlled by association with cyclins (predominantly cyclin B and cyclin A) and by a series of phosphorylation and dephosphorylation events. Activation of CDK1 requires binding to these cyclins, which induce conformational changes that expose the activation loop. Subsequently, phosphorylation at a conserved threonine residue by a CDK-activating kinase (CAK, typically the CDK7–cyclin H–MAT1 complex in mammals) is necessary to stabilize the active conformation. Conversely, inhibitory phosphorylations on residues such as Thr14 and Tyr15, mediated by kinases such as Wee1 and Myt1, maintain the kinase in an inactive state until removed by CDC25 phosphatases. This reversible phosphorylation mechanism ensures that CDK1 activity is precisely coordinated with appropriate cell-cycle events, particularly during the G2/M and early mitosis phases (harper2001cyclindependentkinases pages 2-4, malumbres2005mammaliancyclindependentkinases pages 6-7, sielecki2000cyclindependentkinaseinhibitors pages 2-4, suryadinata2010controlofcell pages 3-4).
7. Function  
   CDK1 plays a pivotal role in controlling eukaryotic cell cycle progression, most notably by driving the G2-M transition and orchestrating mitotic events. It regulates processes such as centrosome duplication, nuclear envelope breakdown, chromosome condensation, spindle assembly, and cytokinesis through phosphorylation of essential substrates. CDK1, when complexed with cyclin B and cyclin A, ensures proper timing and execution of mitosis; for instance, it phosphorylates nuclear lamins to promote nuclear envelope disassembly and modulates microtubule dynamics via phosphorylation of beta-tubulins. Additionally, CDK1 is involved in the regulation of transcription and the DNA damage response by phosphorylating various factors, thereby integrating cell division with broader cellular signaling networks. Its indispensable role in early embryonic development and maintenance of genomic integrity underscores its central function in proliferating cells (brown2015cdk1structuresreveal pages 10-11, harper2001cyclindependentkinases pages 2-4, pluta2024investigatingtherole pages 319-323, poulainUnknownyearinvestigatingp21mediateddynamic pages 147-150, suryadinata2010controlofcell pages 9-10).
8. Other Comments  
   Several small molecule inhibitors have been developed to target CDK1, with RO-3306 being one of the more selective ATP-competitive inhibitors that has been reported. Such inhibitors are of significant therapeutic interest in oncology due to the central role of CDK1 in cell cycle progression and its deregulation in cancer. Alterations in regulatory phosphorylation events or mutations affecting the cyclin-binding interface of CDK1 have been associated with the development of proliferative disorders. CDK1 also undertakes additional roles beyond canonical cell cycle control, including the regulation of transcriptional programs and mitochondrial bioenergetics, making it a multifaceted kinase with diverse cellular impacts (brown2015cdk1structuresreveal pages 1-2, petrone2016identificationofcandidate pages 1-7, wang2023targetingcdk1in pages 8-8, errico2010identificationofsubstrates pages 4-6).
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