2020-06-04

Integrative Structural Model of DNA-PKcs in the Initial Steps of Non-Homologous End Joining

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Title	Integrative Structural Model of DNA-PKcs in the Initial Steps of Non-Homologous End Joining
Institution name	University of Calgary
Expected presentation date	May 2020
Portions	Figure 1
Requestor Location	Mrs. Morgan Hepburn B031A Health Sciences Centre University of Calgary 3330 Hospital Drive N.W. Calgary, AB T2N 4N1 Canada Attn: Mrs. Morgan Hepburn
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J Biol Chem. 2010 Jan 8; 285(2): 1414–1423. PMCID: PMC2801267
Published online 2009 Nov 5. doi: 10.1074/jbc.M109.065615 PMID: 19893054

Ku and DNA-dependent Protein Kinase Dynamic Conformations and Assembly Regulate DNA Binding and the Initial Non-homologous End Joining Complex[*] [S]

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[2]Supported by a graduate scholarship from the Alberta Heritage Foundation for Medical Research and a Canada Graduate Scholarship from the Natural Sciences and Engineering Council of Canada.

Received 2009 Sep 11; Revised 2009 Nov 2

Abstract

DNA double strand break (DSB) repair by non-homologous end joining (NHEJ) is initiated by DSB detection by Ku70/80 (Ku) and DNA-dependent protein kinase catalytic subunit (DNA-PKcs) recruitment, which promotes pathway progression through poorly defined mechanisms. Here, Ku and DNA-PKcs solution structures alone and in complex with DNA, defined by x-ray scattering, reveal major structural reorganizations that choreograph NHEJ initiation. The Ku80 C-terminal region forms a flexible arm that extends from the DNA-binding core to recruit and retain DNA-PKcs at DSBs. Furthermore, Ku- and DNA-promoted assembly of a DNA-PKcs dimer facilitates trans-autophosphorylation at the DSB. The resulting site-specific autophosphorylation induces a large conformational change that opens DNA-PKcs and promotes its release from DNA ends. These results

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J. G. Sheff, M. Hepburn, Y. Yu, S. P. Lees-Miller and D. C. Schriemer, *Analyst*, 2017, **142**, 904
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Author: Joey G. Sheff, David C. Schriemer

Publication: Analytical Chemistry

Publisher: American Chemical Society

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		End Page	1587
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