

DNA **methyl transferases** Enzyme Proteins **CG** specific **Cytosine C5** methylation :

A. **practical**: ChemScape MDL  RasMol  MAGE  FireFox applications.

B. Lunch htdocsLocal <http://aris.gusc.lv/ChemFiles/hhaiDNAmethylCtransferKeny/methmast.htm>

[DNAmethylTransferaseAnswer.doc](#) RSU Aris Kaksis 2025 experimental research **solutions** :

DNA Methyl transferase DNMT3, DNMT1, HhaI: DNMT3 adds methyl groups to **Cytosine** bases in DNA during development of an organism in different types of cells. DNMT1 adds methyl groups to **Cytosine** bases in newly replicated DNA. Hha1 adds methyl groups to DNA in bacterial cells, as part of the restriction/modification system that protects the cell from viruses.

3. N-terminus amino acids is Met1..... and C-terminus amino acid is Tyr327.....

What is total number of amino acids on **6MHT** polypeptide chain 327...?

- Pentose Phosphate backbone** **5. What four bases are a legitimate DNA bases:**
-PO₄- Δ -PO₄- Δ -PO₄- Δ - is ribose Δ **G-Guanine, C-Cytosine, A-Adenine, T-Tyminine**.....
phosphate covalent oxygen ester **6. What four bases are a legitimate RNA bases:**
bonds like bridges. **G-Guanine, C-Cytosine, A-Adenine, U-Uracil**.....
DNA and RNA bases **7. What double stranded DNA sequence recognizes DNMT1 DNA**
G-Guanine-Green **m5c-methyl transferase shown as 3PT6?.... 5'-GCGG-3'**
C-Cytosine-Red **8. What double stranded DNA sequence recognizes HhaI DNA**
A-Adenine-Azure **m5c-methyl transferase shown as 1MHT?.... 5'-GCGC-3'**
T-Tyminine-Tweety bird
U-Uracil-PURple

11. N-terminus amino acid is Met651..... and C-terminus amino acid is Ser1600.....

What is total number of amino acids on **3PT6** polypeptide chain 1600-651+1=950....?

13. What mechanism methylation endogenous or flip out DNA strand **C cytosine**?

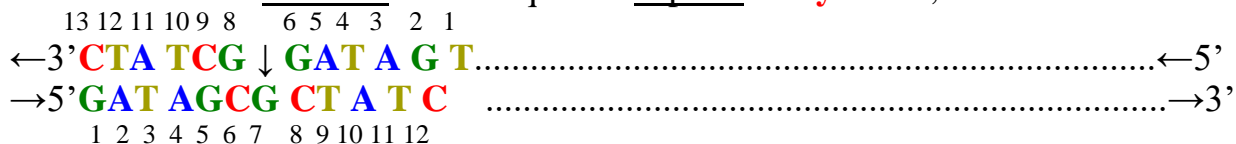
.....flip out DNA strand **C cytosine** (flip out).....

14. What DNA fragment length in **1MHT.pdb** in angstroms? 43.5 Å 42.4 Å .

14a. What base pairs numbers constitute the DNS fragment **1MHT.pdb**?12 base pairs +1.....

14b. Methylation cytosine base number427**C** of DNA fragment **1MHT.pdb** on sequence :

.....427**C** out of DNA sequence flip out **C Cytosine**;



15. What amino acid in before reaction (Equation) bind **cytosine** 427**C** with hydrogen bonds?

residue Glu119... hydrogen bonds start interaction with target 427 **cytosine** .

16. What amino acid with a nucleophilic attack on the sixth cytosine carbon C6 start reaction?

Cys81.... begins with a nucleophilic attack on the sixth cytosine carbon C6 ...

2 Nucl. Acids Res. (1997) 25 (14):2773-2783. © 1997 Oxford University Press **6MHT HhaI**
>6MHT ; 1MHT | P05102 · MTH1_HAEPH Haemophilus parahaemolyticus 327 AA

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1 60
MIEIKDKQLTGLRFIDLFAGLGGFRLALESCGAECVYSNEWDKYAQEVYEMNFGEKPEGD
61 120
ITQVNEKTIPDHDILCAGFPCQAFSISGKQKGFEDSRGTLFFDIARIVREKKPKVVFME
121 180 DNS
VKNFASHDNGNTLEVVKNTMNELDYSFHAKVLNALDYGIPQKRERIYMICFRNDLNIQNF
181 240
QFPKPFELNTFVKDLLLPDSEVEHLVIDRKDLVMTNQEIEQTTPKTVRLGIVGKGGQGER
241 300
IYSTRGIAITLSAYGGGIFAKTGGYLVNGKTRKLRHPRECARVMGYPDSYKVHPSTSQAYK
301 327 360
QFGNSVVINVLQYIAYNIGSSLNFKPY

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2 Science 25 February 2011: Vol. 331 no. 6020 pp. 1036-1040 **human DNA+3PTA human; DMT1**
P26358 DNMT1_HUMAN; 3PTA **646-1600** , 3PT6 **1600-651**

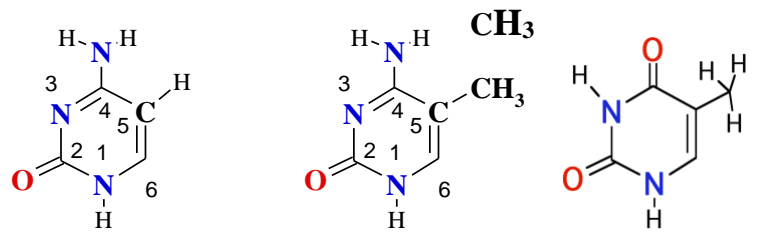
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1 60 70 80
MPARTAPARVPTLAVPAISLPDDVRRRLKDLERDSLTEKECVKEKLNLLHEFLQTEIKNQLCDLETCLRKEELSEEGYLA
81 60 70 160
KVKSLLNKDLSLENGAHAYNREVNGLRENGNQARSEARRVGMADANSPKPLSKPRTPRRSKSDGEAKPEPSPSPRITRK
161 60 70 240
STRQTTITSHFAKGPAPKRPQEESEKAKSDESIKEEDKDQDEKRRRVTSRERVARPLPAEPPERAKSGTRTEKEEERDEK
241 60 70 320
EEKRLRSQTKEPTPKQKLKEEPPDREARAGVQADEDEDGDEKDEKHKRSQPKDLAAKRRPEEKEPEKVNQIISDEKDEDEK
321 60 70 400
EEKRRKTTPKEPTEKKMARAKTMNSKTHPPKCIQCGQYLDDPDLKYQHPPDAVDEPQMLTNEKLSIFDANESGFESYE
401 60 70 480
ALPQHKLTCFVSVKHGHLCPIDTGLIEKNIELFFSGSAKPIYDDDPGLEGGVNGKLNLPINWWITGFDGGEKALIGFS
481 60 70 560
TSFAEYIIMDPSPEYAPIFGLMQEKIYISKIVVEFLQNSDSTYEDLINKIETTVPSPGLNLRFTEDSLLRHAQFVVEQ
561 60 70 640
VESYDEAGDSDEQPIFLTPCMRDLIKLAGVTLGQRRARQARRQTIHSTREKDRGPTKATTTKLVYQIFDTFFAEQIEKDD
641 646 651 720
REDKENAFKRRRCVCEVCQQPECGKCKACKDMVKFGGSGRSKQACQERRCPNMAMKEADDDEEVDNIPEMPSPKKMHQ
721 60 70 800
GKKKKQKNRISWVGEAVKTDGKKSYYKVCIDAETLEVGDVSVIPDDSSKPLYLARVTALWEDSSNGQMFHAHWFCAG
801 60 70 880
TDTVLGATSDPLELFLVDECEMQLSYIHSKVKVIYKAPSENWAMEGGMDPESLLEGDDGKTYFYQLWYDQDYARFESPP
881 60 70 960
KTQPTEDNKFKFCVSCARLAEMRQKEIPRVLEQLEDLDSRVLYSATKNGILYRVGDGVYLPPEAFTFNKLSPPVKRPR
961 60 70 1040
KEPVDEDLYPEHYRKYSDYIKGSNLDAPEPYRIGRIKEIFCPKKSNGRPNETDIKIRVNFYRPENTHKSTPASYHADIN
1041 60 70 1120
LLYWSDEEAVVDFKAVQGRCTVEYGEDLPECVQVYSMGGPNRFYFLEAYNAKSKSFEDPPNHARSPGNKGGKGGKGGKGP
1121 60 70 1200
KSQACEPSEPEIEIKLPLKRLTDLVDFSGCGLSEGFHQAGISDTLWAIEMWDPAAQAFRLNPNPGSTVFTEDCNILLKLVMA
1201 60 70 1360
GETTNSRGQRLPQKGDVEMLCGGPPCQGFSGMNRFNRSRTYSKFNLSVLSFLSYCDYRPRFFLENVRNFVSKRSMVL
1361 60 70 1440
KLTLRCLVRMGYQCTFGVLQAGQYGAQTRRRRAIILAAAPGEKPLPFPEPLHVFAPRACQLSVVDDKFKVSNITRLSSG
1441 60 70 1520
PFRTITVRDMSDLPEVRNGASALEISYNGEPQSWFQRQLRGAQYQPILRDHICKDMSALVAARMRHIPLAPGSDWRDLF
1521 60 70 1600
NIEVRLSDGTMARKLRYTHHDRKNGRSSSGALRGVCSCEVAGKACDPAARQFNTLIPWCLPHTGNRHNHWAGLYGRLEWD
1601 60 70 1680
GFFSTTVTNPEPMGKQGRVLHPEQHRVSVRECARSQGFPTYRLFGNILDKHRQVGNVPPPLAKAIGLEIKLCMLAKA
1681 1691 1697
RESASAKIKEEEAAKD
HETNAM SAH S-ADENOSYL-L-HOMOCYSTEINE ZN ZINC ION
FORMUL 4 SAH C14 H20 N6 O5 S
FORMUL 5 ZN 4(ZN 2+)

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17. Put in **C**, **m5C** **C** and **T**

heterocyclic structures nitrogen atoms **1N**, **3N**, and side amino group **H₂N-4** at carbon **4C**, oxygen **=O**. Put in Methyl group **-CH₃** mc5 cytosine to carbon **5C**!



O
(Equation) **C**

m5C**C**

T

18. Put in **S⁺**-adenosyl-L-

methionine with short cut

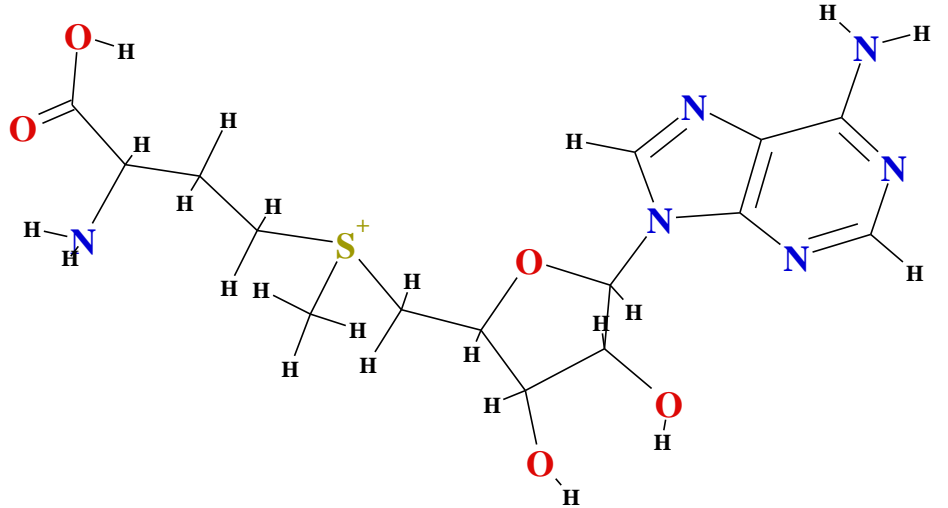
name AdoMet five **N** atoms

and methyl sulfur **S⁺**-called

AdoMet! Put in two ribose

oxygen atoms at **C2** and **C3**

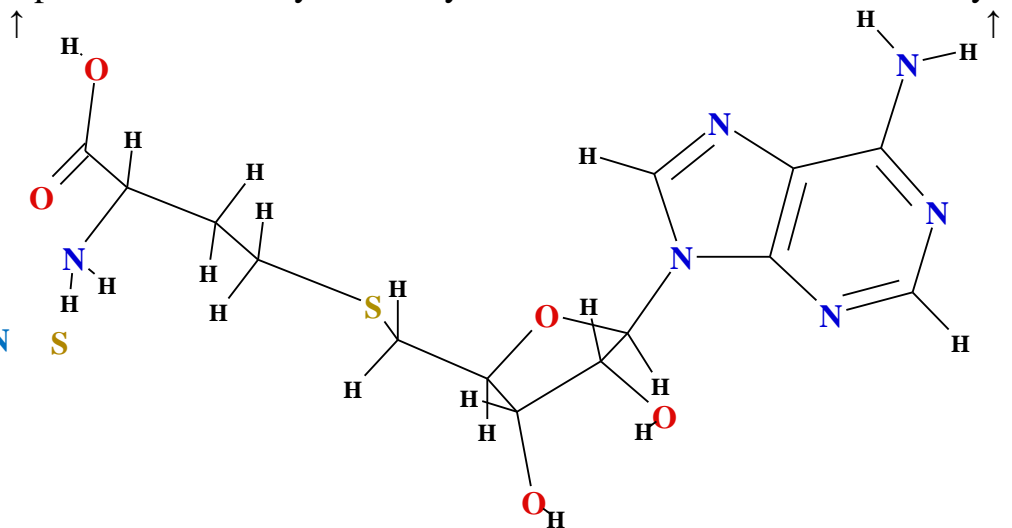
of molecule!



19. Put in **C** and **A** methylation product **S**-adenosyl homo cysteine with short cut name AdoHcy!

Put in five **N** atoms and sulfur **S**-adenosyl homo cysteine connected to ribose carbon atom **C5**!

Put in two ribose oxygen atoms at **C2** and **C3** of molecule!



N N N N N S

O O

20. Choose on left frame button [Protein](#) and MDL (select Mouse click Action) distance to

measure 3D size of **1MHT.pdb** molecule in angstroms? 76.5 Å.....59.6 Å40.7 Å

21. What three domains connected by **1MHT-6MHT.pdb** methyl transferase?

large domain and.....**small domain**,.....connected by.....a **hinge region**.....

22. Between what is located pronounced cleft in **hinge region**?

between the **large domain** and **small domain** ..

23. What four **DNA** base pairs are capable bound the cleft in **hinge region**?

cleft is capable binding double stranded **B-DNA** at 5'-**GCGC**-3'

..... 3'-**CGCG**-5'.....

24. What type secondary structures dose contains the **large domain** of methyl transferase?

..... **beta** structure and**alpha helices**.

25. Choosing by right button “select’ and “Highlight Selection” what **beta sheets** and how many **beta strands** constitute methyl transferases and what position of **hairpin-loop**?
beta sheet one..... with.....**five parallel** and one..... **strand with hairpin-loop**.
26. What **alpha helices** constitute methyl transferase molecule? sandwich between **two**.....
alpha helices plus one.....**beta strand as butter** between **second two**.....**alpha helices**
and one..... **alpha helix** that lies.....in front of the **beta sheet core**
27. What type secondary 2° structures dose contains the **small domain** of methyl transferase?
one..... as **beta sheet**.
28. What **beta sheets** and how many **beta strands** constitute methyl transferase molecule?
five.....**beta strands** are configured in an anti parallel formation.
and are arranged in a circular formation that resembles a pinwheel..... (spirālveida ritenis)
29. What secondary structures dose contains the **hinge region** of methyl transferase?
hinge region is composed of an **alpha-loop-alpha**..... structure
that connects the **large**..... **domain** with.....**small domains**
30. What conserved motifs comprise **hinge region** of methyl transferase?
hinge region is comprised with IX.....and.....X conserved motifs
the first half motif IX **small**.....**domain** second half X locates in **large**.....**domain**
31. What conserved motifs labeled **variable region** spans the entire length of the methyl transferase?**variable region** between VIII.....and IX.....motifs
32. What two units within **variable region** between VIII and IX motifs of methyl transferase
responsible for sequence 5'-**GCGC**-3’ specific recognition and?
target base selection recognition **domain** to **small**.....**sub region**
33. What twenty six amino acids bind AdoMet in site a **hydrophobic pocket**?.....
5AA: Phe18.....,Ala19.....,Gly20.....,Leu21.....,Gly22....., 11: Gly23.....,Phe24.....,Ala27.....,Trp41.....,
Pro57.....,Gly59.....,Ile61.....,Ile74.....,Cys76.....,Ala77.....,Gly78....., 10: Phe79.....,Pro80.....,Gly98.....,
Leu100.....,Phe101.....,Phe102.....,Val121.....,Val115.....,Val306.....,Val307.....

38. What type methyl transferase adds **methyl** groups to **Citozīns** bases in DNS in bacterial cells, as part of the restriction/modification system that protects the cell from viruses?

Hha1-1MHT.pd,6MHT.pdb.....

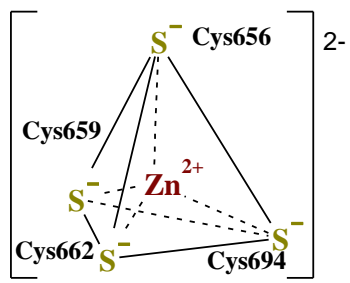
39. What type methyltransferase adds **methyl** groups to **Cytosine** bases in DNA in newly replicated DNA. These **methyl** groups are important for replicating controlling genes in different types of newly reproducing cells copies? ... **DNMT1-3PT6.pdb**.....

40. What type methyltransferase adds **methyl** groups to **Cytosine** bases in DNA during development of an organism cell. These **methyl** groups are important for **epigenetic** controlling genes in differentiation development of cell types? ... **DNMT3-2QRV.pdb**.....

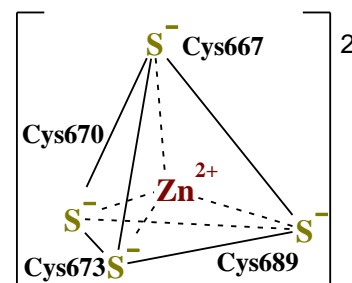
Fresh replicate DNA methylase DNMT1 PDB 3PT6

41. What four amino acids in **zinc(II)** ion finger coordination sphere **Zn2** and **Zn4** **3PT6.pdb**?
Cys656.....Cys659.....Cys662.....Cys694.....; Zn4 Cys667.....Cys670.....Cys673.....Cys689.....

42. Put in **Zn²⁺**
 coordinative Geometry
 Tetragon Nr2 with 4 sulfur
S⁻ ions and complex charge!
3PT6Zn2

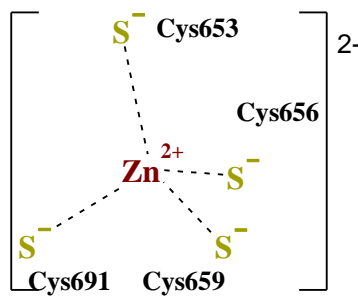


43. Put in **Zn²⁺**
 coordinative
 Geometry Tetragon
 Nr4 with 4 sulfur **S⁻**
 ions and complex
 charge! **3PT6Zn4**
S⁻ S⁻ S⁻ S⁻ 2-

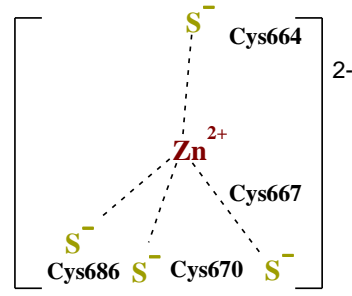


44. What four amino acids in **zinc(II)** ion finger coordination sphere **Zn2** and **Zn5** **3PTA.pdb**?
Cys653-Cys656-Cys659-Cys691-.....Cys667-Cys670-Cys673-Cys689-

45. Put in **Zn²⁺**
 coordinative Geometry
 Tetragon Nr2 with
 4 sulfur **S⁻** ions and
 complex charge!
3PTAZn2



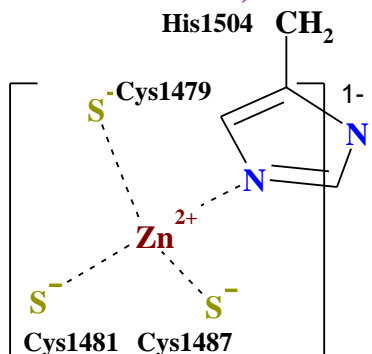
46. Put in **Zn²⁺**
 coordinative Geometry
 Tetragon Nr5 with
 4 sulfur **S⁻** ions and
 complex charge!
3PTAZn5



47. What four amino acids in **zinc(II)** ion finger coordination sphere **Zn1702-1703** **4DA4.pdb**?
Zn1702 Cys1479.....Cys1481.....Cys1487.....His1504.....;

; Zn²⁺ 1703 HIS796.....Cys823.....Cys897.....Cys900.....

48. Put in **Zn²⁺**
 coordinative
 Geometry
 Tetragon Nr1702
 with 3 sulfur **S⁻** ions,
 His1504 two **N**
 atoms and complex
 charge!
4DA4Zn1702



49 Put in **Zn²⁺**
 coordinative
 Geometry Tetragon
 Nr1703 with
 3 sulfur **S⁻** ions,
 His796 two **N** atoms
 and complex charge!
4DA4Zn1703

