**Table S1**. Details of known methyltransferases of *Arabidopsis* and rice.

| **Gene_name** | **Gene identifier** | **Chromosome** | **Gene length (bp)** | **Protein length (aa)** |
|---|---|---|---|---|
| ***Arabidopsis thaliana*** | | | | |
| *AtCMT1* | AT1G80740 | Chr1 | 4655 | 791 |
| *AtCMT2* | AT4G19020 | Chr4 | 6684 | 1295 |
| *AtCMT3* | AT1G69770 | Chr1 | 5268 | 839 |
| *AtMET2* | AT4G14140 | Chr4 | 5787 | 1545 |
| *AtMET3* | AT4G13610 | Chr4 | 6210 | 1404 |
| *AtMETIIb* | AT4G08990 | Chr4 | 5716 | 1512 |
| *AtMET4/AtDDM2* | AT5G49160 | Chr5 | 6140 | 1534 |
| *AtDRM1* | AT5G15380 | Chr5 | 3480 | 624 |
| *AtDRM2* | AT5G14620 | Chr5 | 3452 | 626 |
| *AtDRM3* | AT3G17310 | Chr3 | 4242 | 710 |
| *AtDNMT2* | AT5G25480 | Chr5 | 2390 | 383 |
| ***Oryza sativa*** | | | | |
| *OsMET1* | LOC_Os03g58400 | Chr3 | 2245 | 376 |
| *OsMET2* | LOC_Os07g08500 | Chr7 | 2298 | 377 |
| *OsCMT1* | LOC_Os03g12570 | Chr3 | 11118 | 1787 |
| *OsCMT2* | LOC_Os05g13780 | Chr5 | 13681 | 1407 |
| *OsCMT3* | LOC_Os10g01570 | Chr10 | 5284 | 371 |
| *OsDRM1a* | LOC_Os11g01810 | Chr11 | 4216 | 473 |
| *OsDRM2* | LOC_Os03g02010 | Chr3 | 3700 | 507 |
| *OsDNMT2* | LOC_Os01g42630 | Chr1 | 2248 | 280 |

**Table S2.** List of primers used in this study.

| **Primers for cloning in pUC based 35S-psGFPs-tNOS vector** | |
|---|---|
| **Gene name** | **Primer sequence** |
| *CaCMT1*_F | 5’-ATAGGGCCCATGATCCAGAATG-3’ |
| *CaCMT1*_R | 5’-AATCCCGGGTCAAAGAATAGGA-3’ |
| *CaDRM1*_F | 5’-TTAGGGCCCATGGGTGATGTT-3’ |
| *CaDRM1*_R | 5’-AATCCCGGGTCTATAATTTGGTGA-3’ |
| *CaMET1*_F | 5’-AATGGGCCCATGTTCAAAACAG-3’ |
| *CaMET1*_R | 5’-ATACCCGGGTCATCTGTTTCTTG-3’ |
| **Primers for quantitative real-time PCR** | |
| **Gene name** | **Primer sequence** |
| *CaCMT2*_F | 5’-GGAGATCCGATTTCCGATGA-3’ |
| *CaCMT2*_R | 5’-GATGGCTTCTTTTCCTTTTCTTGA-3’ |
| *CaCMT1*_F | 5’-GTTGCAGCTGGGTGTTATGGT-3’ |
| *CaCMT1*_R | 5’-GGGTAGAACCTCGTCAGGATGA-3’ |
| *CaCMT3*_F | 5’-TGACAAGAGCAGAGCCTCACA-3’ |
| *CaCMT3*_R | 5’-TTTCACGTATGCTAAGAACTCGATCT-3’ |
| *CaDNMT2*_F | 5’-GTGCTGATGCATGGCTTCTTT-3’ |
| *CaDNMT2*_R | 5’-CCAGTGTCCTTCTGGAGACCTT-3’ |
| *CaDRM1*_F | 5’-CATGATGCATTTCCACTGTTGA-3’ |
| *CaDRM1*_R | 5’-TTCCAGTGACCGTTTGCAAA-3’ |
| *CaDRM2*_F | 5’-GGGTTTTTGATCTGGTCATTTATCA-3’ |
| *CaDRM2*_R | 5’-AAGCTGAGAGACTTCCAATGGTATG-3’ |
| *CaMET1*_F | 5’-CGCCCAAATAGAAGAATTACAGACTT-3’ |
| *CaMET1*_R | 5’-GTCCGGTGATAAACAAATCGTTAA-3’ |
| *Ca-EF1α*_F | 5’-TCCACCACTTGGTCGTTTTG-3’ |
| *Ca-EF1α*_R | 5’-CTTAATGACACCGACAGCAACAG-3’ |

**Table S3**. Details of methyltransferases identified in three legumes and grapevine.

| Gene_name | Gene identifier | Chromosome | Gene length (bp) | Protein length (aa) |
|---|---|---|---|---|
| ***Medicago truncatula*** | | | | |
| *MtCMT1* | Medtr5g023660.1 | Chr5 | 5816 | 835 |
| *MtCMT2* | Medtr5g066780.1 | Chr5 | 2810 | 800 |
| *MtCMT3* | AC233109_38.1 | - | 5550 | 827 |
| *MtMET1* | Medtr4g035150.1 | Chr4 | 8048 | 1641 |
| *MtMET2* | Medtr6g065580.1 | Chr6 | 9053 | 1573 |
| *MtDRM1* | Medtr3g011150.1 | Chr3 | 6403 | 628 |
| *MtDRM2* | Medtr5g019420.1 | Chr5 | 8781 | 751 |
| *MtDRM3* | Medtr6g005580.1 | Chr6 | 9837 | 588 |
| *MtDRM4* | AC235665_42.1 | - | 6403 | 628 |
| *MtDNMT2a* | Medtr2g009140.1 | Chr2 | 4840 | 378 |
| *MtDNMT2b* | Medtr5g066830.1 | Chr5 | 579 | 192 |
| *MtDNMT2c* | Medtr8g062560.1 | Chr8 | 935 | 151 |
| ***Lotus japonicus*** | | | | |
| *LjCMT1* | chr2.CM0065.100.nd | Chr2 | 7880 | 866 |
| *LjCMT2* | chr4.CM0680.70.nc | Chr4 | 8536 | 900 |
| *LjCMT3* | LjT31J09.230.nd | - | 9005 | 536 |
| *LjCMT4* | LjSGA_028177.1 | - | 1805 | 774 |
| *LjMET1* | chr2.CM0272.410.nd | Chr2 | 3618 | 416 |
| *LjMET2* | chr3.LjB23H05.80.nd | Chr3 | 6927 | 1534 |
| *LjDRM1* | chr2.CM0008.250.nc | Chr2 | 3243 | 440 |
| *LjDRM2* | LjB15A13.10.nd | | 9940 | 606 |
| *LjDNMT2a* | chr6.CM0055.800.nd | Chr6 | 1516 | 328 |
| *LjDNMT2b* | LjSGA_133586.1 | - | 449 | 147 |
| *LjDNMT2c* | LjSGA_015229.1 | - | 1824 | 138 |
| *LjDNMT2d* | LjSGA_084646.1 | - | 324 | 107 |
| ***Cajanus cajan*** | | | | |
| *CcCMT1* | C.cajan_12460 | Chr6 | 5744 | 822 |
| *CcCMT2* | C.cajan_15419 | Chr8 | 5748 | 723 |
| *CcCMT3* | C.cajan_04198 | Chr11 | 18095 | 893 |
| *CcMET1* | C.cajan_32735 | Scaffold | 6394 | 1290 |
| *CcDRM1* | C.cajan_12070 | Chr6 | 2128 | 411 |
| *CcDNMT2a* | C.cajan_17086 | Chr8 | 4156 | 384 |
| *CcDNMT2b* | C.cajan_28099 | Scaffold | 1796 | 344 |
| ***Vitis vinifera*** | | | | |
| *VvCMT1* | GSVIVT01022685001 | Chr2 | 32565 | 729 |
| *VvCMT2* | GSVIVT01025386001 | Chr6 | 13286 | 821 |
| *VvCMT3* | GSVIVT01033464001 | Chr8 | 5897 | 827 |
| *VvCMT4* | GSVIVT01024446001 | Chr16 | 42296 | 847 |
| *VvMET1* | GSVIVT01000262001 | Chr7 | 6078 | 1417 |
| *VvMET2* | GSVIVT01000263001 | Chr7 | 9060 | 1429 |
| *VvDRM1* | GSVIVT01032445001 | Chr14 | 13086 | 512 |
| *VvDNMT2a* | GSVIVT01035808001 | Chr4 | 4998 | 366 |
| *VvDNMT2b* | GSVIVT01023152001 | Chr12 | 6707 | 460 |
| *VvDNMT2c* | GSVIVT01023383001 | Chr12 | 294 | 74 |
| *VvDNMT2d* | GSVIVT01022824001 | Chr12 | 2035 | 83 |
| *VvDNMT2e* | GSVIVT01023370001 | Chr12 | 1908 | 60 |

**Table S4**. Nuclear localization signal predicted in chickpea and soybean methyltransferases.

| **Protein name** | **Position (aa)** | **NLS sequence** | **Score** | **Monopartite/ bipartitite** |
|---|---|---|---|---|
| CaCMT1 | 93 | GNPPKKKYKTS | 9 | monopartite |
| CaCMT2 | 187 | EPKRVFFSEVQDDNPLDCLVEKLNIARLP | 4.3 | bipartite |
|  | 221 | DAKKKVIPPCDYYCDTLYLLPYSTFVKLPSES | 4.4 | bipartite |
| CaCMT3 | 25 | LPSQRKKAKHS | 8.5 | monopartite |
|  | 6 | FSMGKRAQQSPQNDDVVSLLPSQRKKAKHS | 7.3 | bipartite |
| CaMET1 | 30 | NKKKRNSSESSEQPAPTRKMPKRS | 11.8 | bipartite |
| CaDRM1 | 325 | RKRGYIHNLPIENRYPLLPLPPRTIHDA | 6 | bipartite |
| CaDRM2 | 305 | DRNKRPKYEY | 5.5 | monopartite |
| CaDNMT2 | 285 | VYPDSKRCCCFTKSY | 6 | monopartite |
| GmCMT1 | 8 | PSKRKTRSSASPAAAPPSKRASRS | 9.4 | bipartite |
| GmCMT2 | 28 | LPSQRKKPKHS | 9.5 | monopartite |
|  | 9 | KKRSASDATDDAQNDTVSLLPSQRKKPK | 7 | bipartite |
| GmCMT3 | 53 | RYATMAKRKTSDASDAQDDTVSLLPSQRNKAKHP | 6.2 | bipartite |
|  | 204 | DLVDKKRIFISDVKDVNPLDCIVSKVKIYKKS | 6.6 | bipartite |
| GmCMT4 | 340 | NRFRNCASPLDDERNRQIVIFMDMVKFLKP | 6.1 | bipartite |
| GmMET1 | 43 | DKQKKRSLSESSEQTAAMRKMPKR | 10 | bipartite |
| GmMET2 | 43 | DKQKKRSLLESSEQPAATRKMPKR | 9.6 | bipartite |
| GmDRM1 | 264 | RKRGYIHNLPTHNRSPLLPIPPLTIQEA | 5.3 | bipartite |
| GmDRM2 | 212 | KSNKRRLYDYEVLGRKKPRG | 13.7 | bipartite |
| GmDRM3 | 330 | GRGKRPKYE | 7 | monopartite |
| GmDRM4 | 365 | GRGKRPKYE | 7 | monopartite |
| GmDRM5 | 201 | KSNKRRFYDYEVLGRKKPRG | 12.3 | bipartite |
| GmDNMT2a | 96 | RPRYFCLAKRKPSSFVNECLNNLLIQSSPPLFGHFD | 4.4 | bipartite |
| GmDNMT2b | 295 | VYPDSKRCCCFTKSY | 6 | bipartite |

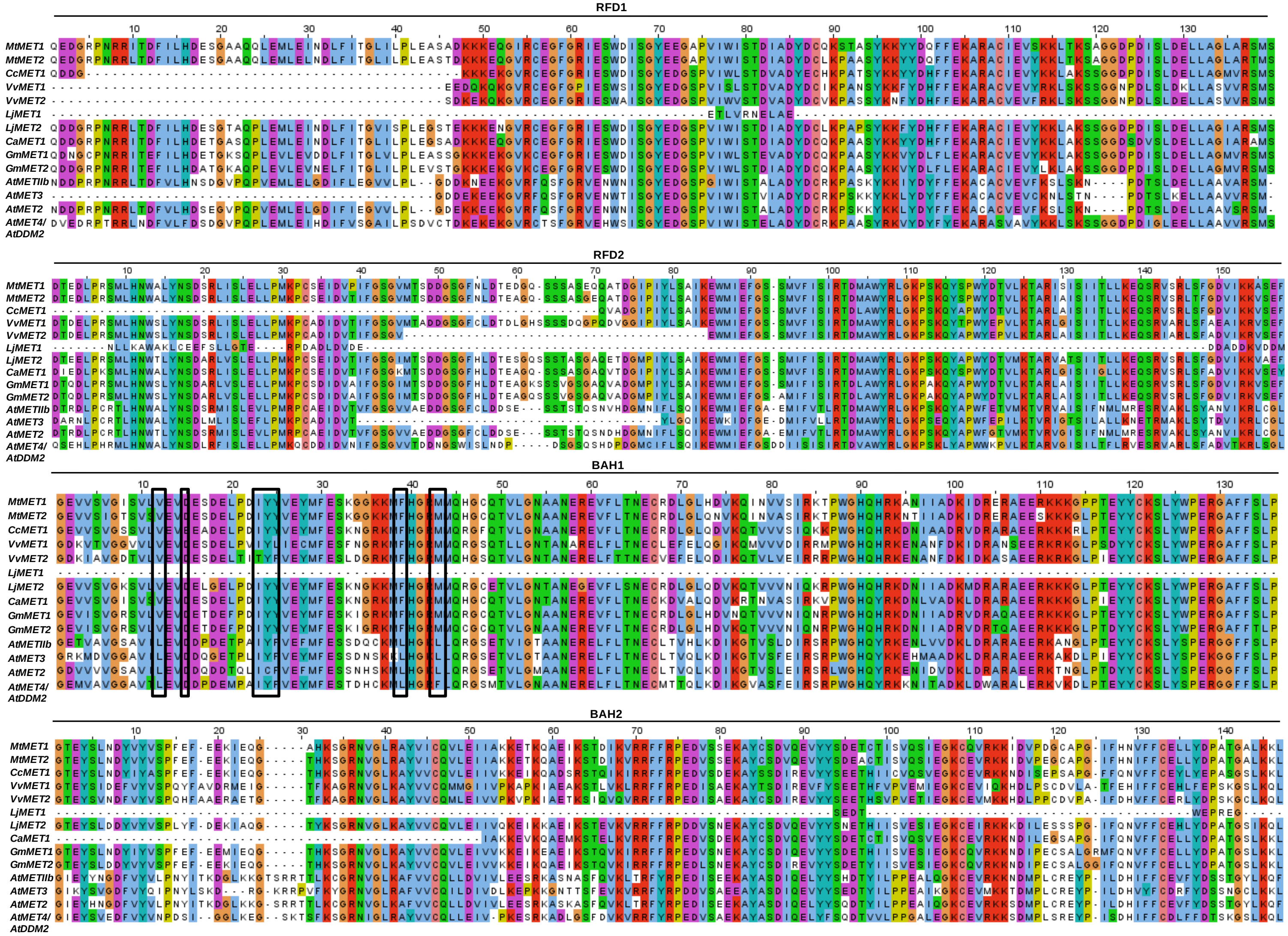
**Table S5**. Summary of homology modeling statistics of representative members of soybean and chickpea methyltransferases.

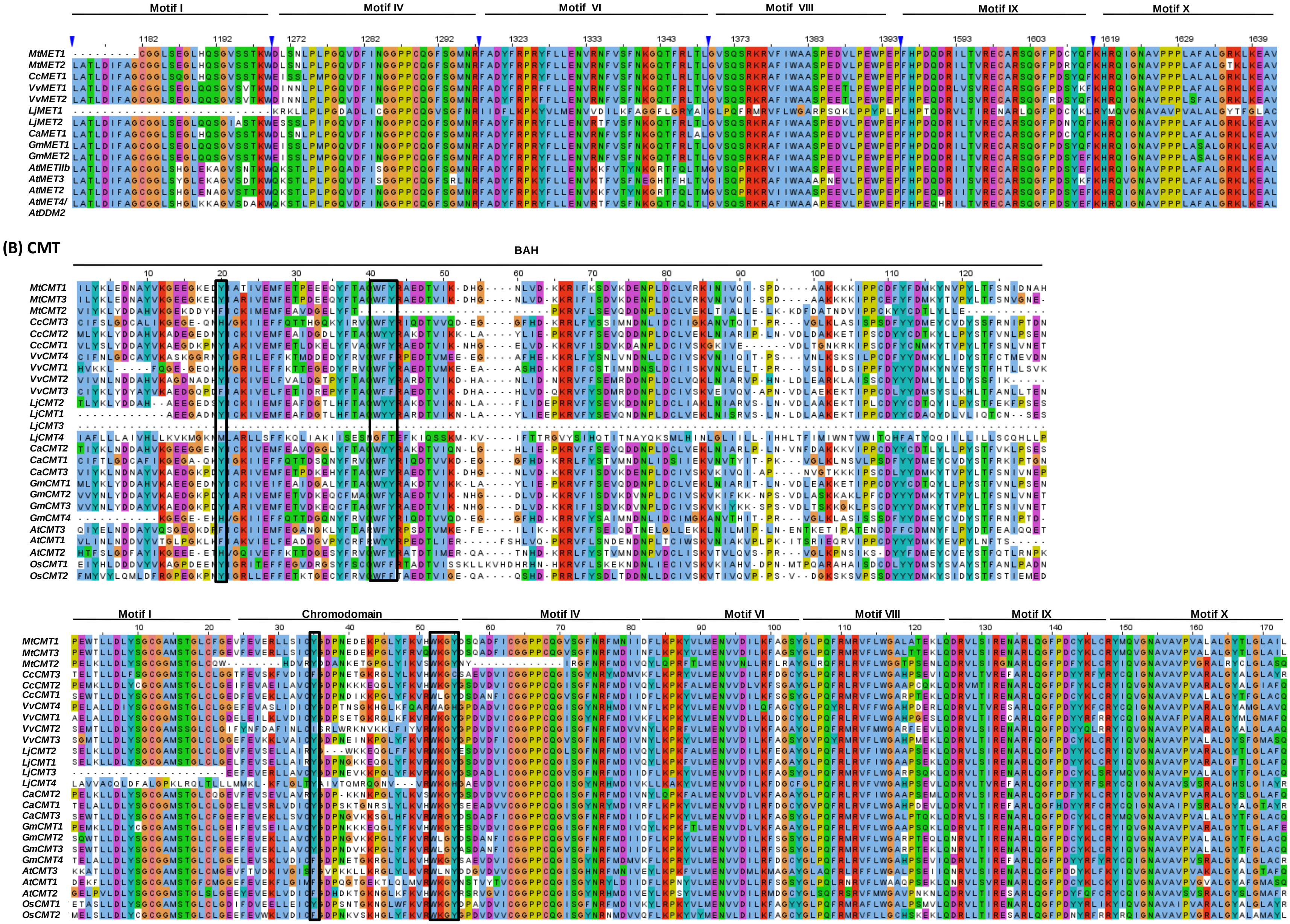
| **Protein name** | **Template used for homology modelling (PDB ID)** | **Identity (%)** | **Query Coverage (%)** | **Residues in favoured region (%)** | **Residues in allowed regions (%)** | **Residues in outlier regions (%)** | **RMSD (Å)** |
|---|---|---|---|---|---|---|---|
| **CaCMT2** | 4FT2 | 53 | 90 | 86.1 | 7.9 | 6.0 | 0.549 |
| **CaCMT2** | 4FT4 | 53 | 90 | 88.9 | 6.6 | 4.5 | 0.905 |
| **CaMET1** | 3AV4 | 42 | 84 | 90.1 | 6.6 | 3.4 | 3.09 |
| **CaDRM1** | GmDRM5 | 81 | 100 | 86.4 | 6.6 | 7.0 | 0.184 |
| **CaDNMT2** | 1G55 | 37 | 97 | 90.2 | 6.9 | 2.9 | 0.211 |
| **GmCMT2** | 4FT2 | 55 | 94 | 84.5 | 10.5 | 5.0 | 0.417 |
| **GmCMT2** | 4FT4 | 55 | 94 | 88.7 | 7.8 | 3.5 | 0.603 |
| **GmMET2** | 3AV4 | 31 | 93 | 89.7 | 6.8 | 3.5 | 3.43 |
| **GmDRM5** | Threading[1] | - | - | 86.5 | 5.4 | 8.1 | - |
| **GmDNMT2a** | 1G55 | 38 | 96 | 90.3 | 6.3 | 3.4 | 0.210 |

[1] 78% residues modeled with more than 90% confidence.

**Figure S1**. **Multiple sequence alignment of all the classes of MTases identified in legumes.** Multiple sequence alignments were generated using JalView to highlight the conserved domains (line on top of alignments) and residues (black rectangular boxes) in MET (A), CMT (B), DRM (C) and DNMT2 (D).

**(A) MET**





Motif I
Motif IV
Motif VI
Motif VIII
Motif IX
Motif X
1182
1192
1272
1282
1292
1323
1333
1343
1373
1383
1393
1593
1603
1619
1629
1639
MtMET1
MtMET2
CcMET1
VvMET1
VvMET2
LjMET1
LjMET2
CaMET1
GmMET1
GmMET2
AtMETIIb
AtMET3
AtMET2
AtMET4/
AtDDM2
(B) CMT
BAH
10
20
30
40
50
60
70
80
90
100
110
120
MtCMT1
MtCMT3
MtCMT2
CcCMT3
CcCMT2
CcCMT1
VvCMT4
VvCMT1
VvCMT2
VvCMT3
LjCMT2
LjCMT1
LjCMT3
LjCMT4
CaCMT2
CaCMT1
CaCMT3
GmCMT1
GmCMT2
GmCMT3
GmCMT4
AtCMT3
AtCMT1
AtCMT2
OsCMT1
OsCMT2
Motif I
Chromodomain
Motif IV
Motif VI
Motif VIII
Motif IX
Motif X
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
MtCMT1
MtCMT3
MtCMT2
CcCMT3
CcCMT2
CcCMT1
VvCMT4
VvCMT1
VvCMT2
VvCMT3
LjCMT2
LjCMT1
LjCMT3
LjCMT4
CaCMT2
CaCMT1
CaCMT3
GmCMT1
GmCMT2
GmCMT3
GmCMT4
AtCMT3
AtCMT1
AtCMT2
OsCMT1
OsCMT2

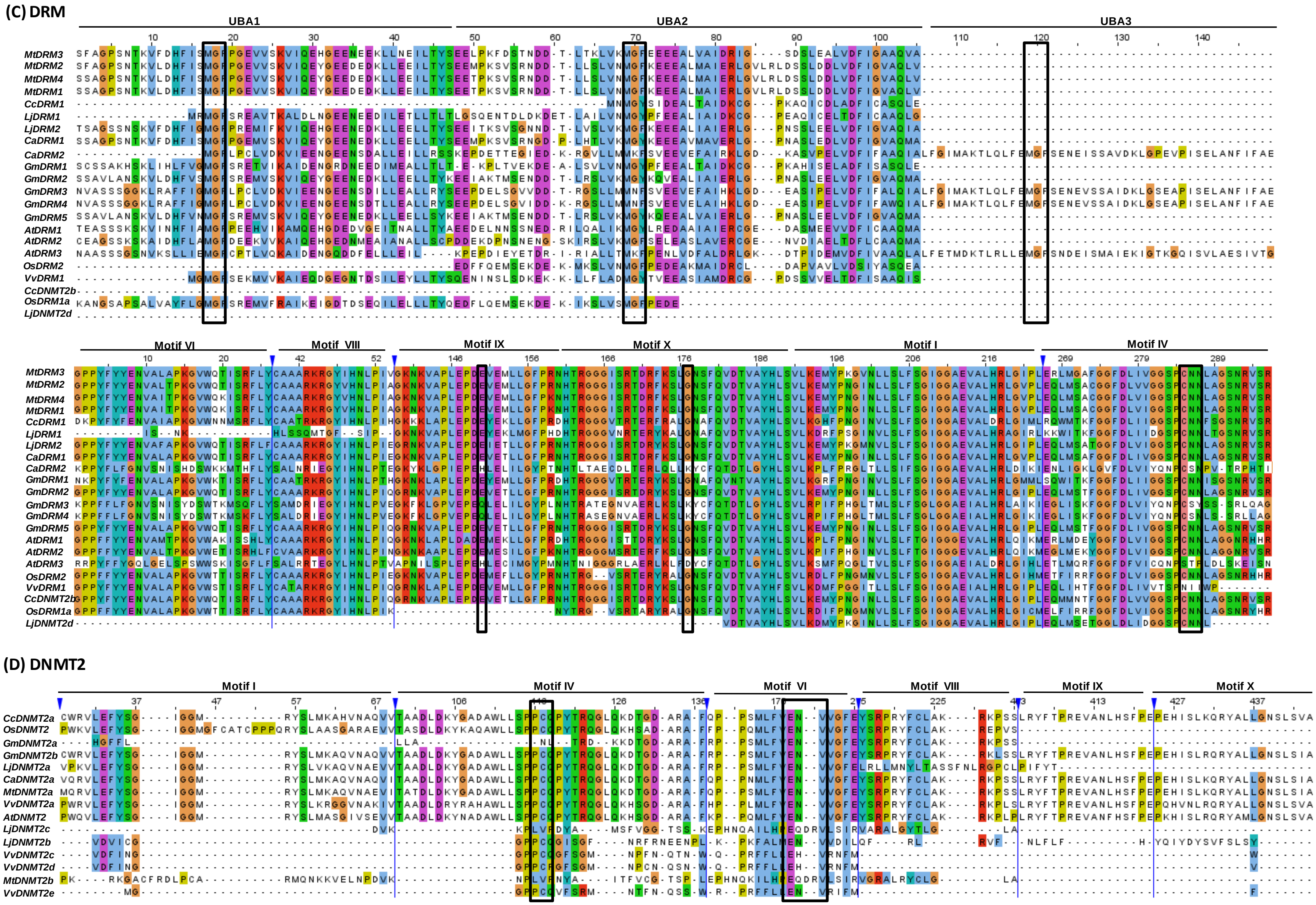

(C) DRM
UBA1
UBA2
UBA3
MtDRM3
MtDRM2
MtDRM4
MtDRM1
CcDRM1
LjDRM1
LjDRM2
CaDRM1
CaDRM2
GmDRM1
GmDRM2
GmDRM3
GmDRM4
GmDRM5
AtDRM1
AtDRM2
AtDRM3
OsDRM2
VvDRM1
CcDNMT2b
OsDRM1a
LjDNMT2d
Motif VI
Motif VIII
Motif IX
Motif X
Motif I
Motif IV
(D) DNMT2
Motif I
Motif IV
Motif VI
Motif VIII
Motif IX
Motif X
CcDNMT2a
OsDNMT2
GmDNMT2a
GmDNMT2b
LjDNMT2a
CaDNMT2a
MtDNMT2a
VvDNMT2a
AtDNMT2
LjDNMT2c
LjDNMT2b
VvDNMT2c
VvDNMT2d
MtDNMT2b
VvDNMT2e

**Figure S2**. **Three-dimensional (3D) structures of soybean and chickpea CMT proteins constructed by homology modeling.** Ribbon representation of GmCMT2 and CaCMT2 protein structures with bound H3(1–15)K9me2 peptide. The BAH, methyltransferase, and Chr domains are colored in red, cyan, and blue, respectively, with bound S-adenosylhomocysteine (SAH) molecule (orange) and H3(1–15)K9me2 peptide (yellow, bound to Chr domain) shown in a space filling representation. The K9me2 is accommodated within an aromatic cage formed by Tyr400, Phe370 and Trp397in GmCMT2 and by Tyr415, Trp431 and Tyr434 in CaCMT2 (*Inset*). Intermolecular hydrogen bonds between H3K9me2 peptide and Chr domain are designated by dashed lines (*Inset*).

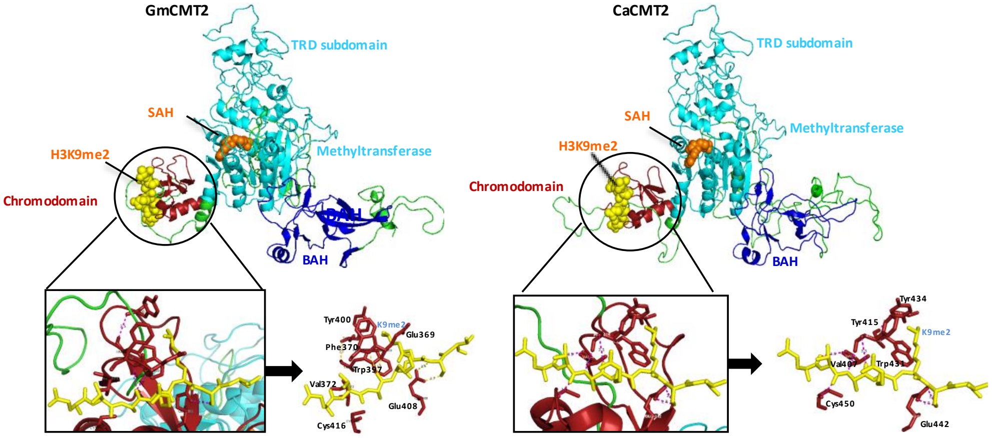


**Figure S3**. **Structural features of plant METs.** (A) The RFD domain pluged into the DNA-binding pocket. The RFD domain (magenta) is positioned in the DNA-binding pocket (cyan) of MET and stabilized by several hydrogen bonds (inset; yellow dashed lines) or non-bonded interactions (inset; interacting residues shown as sticks) with the catalytic domain. PCQ region of the catalytic domain is highlighted in red color. (B) Comparison of the TRD subdomain of MET with CMT. Comparison of the TRD subdomains of MET (purple) and CMT (cyan) by superimposing their structures. The regulatory region of TRD subdomain in CMTs is occupied by two antiparallel sheets (arrow), whereas only loop is present in MET indicative of different regulatory mechanisms in these MTases. Chromodomain is shown in red color.

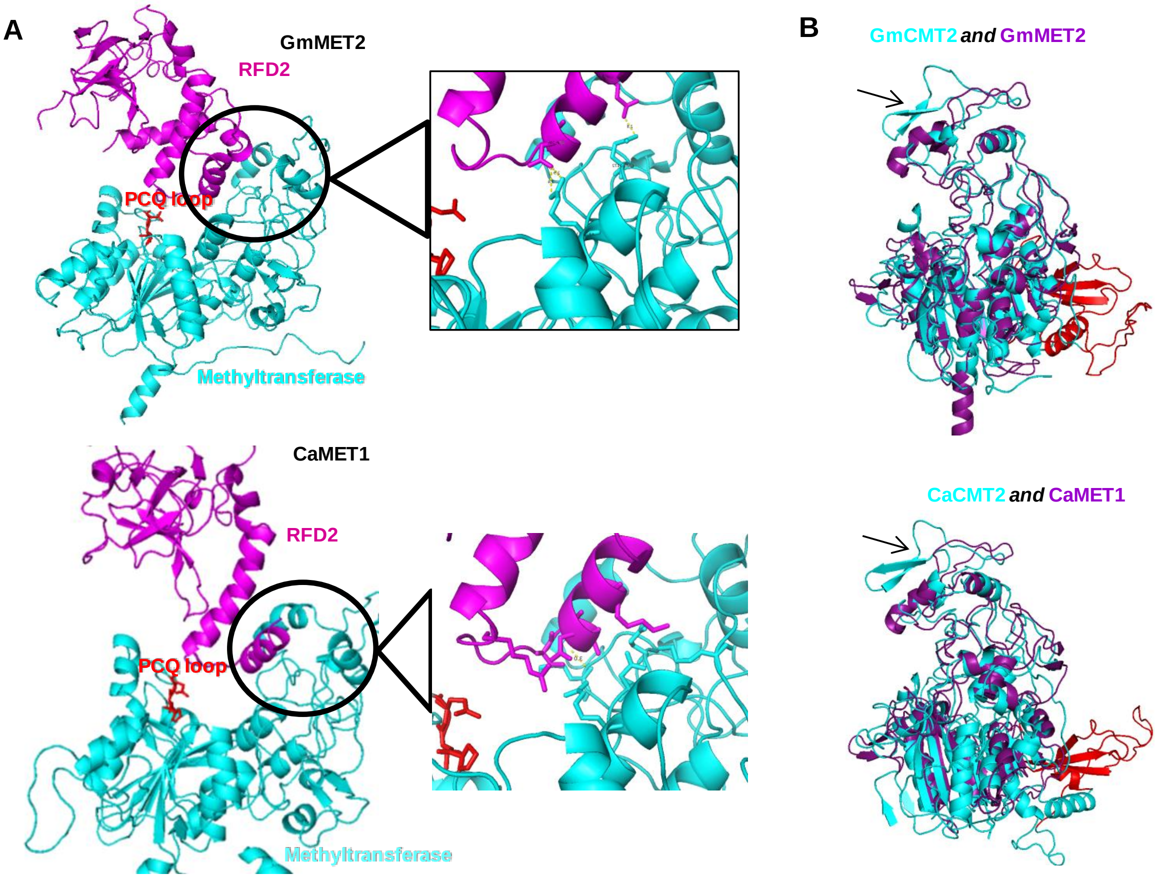
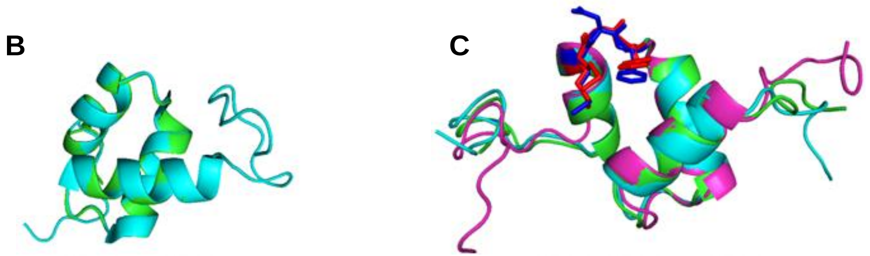


**Figure S4. Structural features of plant DRMs.** (A) Ribbon representation of the structure of CMT with bound SAH to motif I (magenta) and motif X (red). Bound SAH molecule shown in a space filling representation. (B) The UBA domains (UBA1 and UBA2) are colored in cyan and green. (C) Comparison of UBA1 (cyan), UBA2 (green) and UBA3 (magenta) structures with conserved MGF/MGY shown as sticks.

GmCMT2 - **Motif I** and **Motif X** forming SAH binding cleft



**UBA1** and **UBA2**

**UBA1**, **UBA2** and **UBA3**