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Supporting information for article:

**Crystal structure of Rv1220c, a SAM-dependent O-
methyltransferase from *Mycobacterium tuberculosis***

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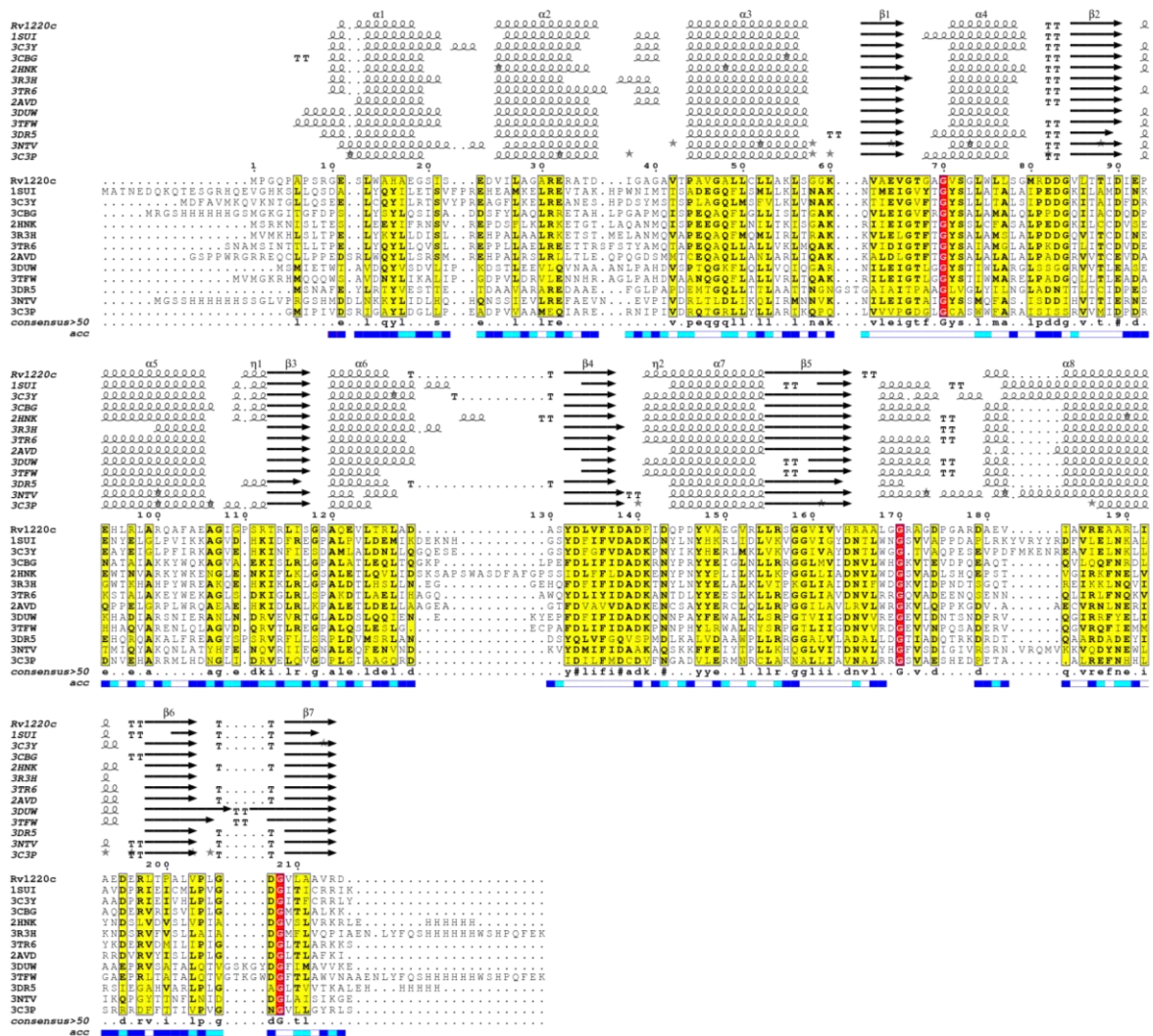


Figure S1 Alignment of primary sequences of structural homologues of *MtbOMT*. PDB codes of corresponding homologous structures are listed in the column on left. Absolutely conserved amino acids are highlighted in red, conserved amino acids are highlighted in yellow. The secondary structural elements of all the homologues are marked.

M.tuberculosis	1MP.....GQFAPSR
M.bovis	1MP.....GQFAPSR
M.canettii	1MP.....GQFAPSR
M.marinum	1MSRRHSWQRARLPDCVANPTYAAGMHGTDSSSDTP..GQFAPSR
M.liflandii	1MSRRHSWQRARLPDCVANPTYAAGMHGTDSSSDTP..GQFAPSR
M.ulcerans	1MHGTDSSSDTP..GQFAPSR
M.triplex	1MQY..LAGMDGSDETP..GQAVPSR
M.genavense	1MDGSDETP..GQVAPSR
M.leprae	1MYGTGNNAVTP..DAAA SR
M.avium	1MDGTDAEAP..GQTAPSR
M.colombiense	1MDGTDAEAP..GQTAPSR
M.kansasii	1	MTFITRRIPGVSAARCRPRSGHRARLPDGVADPAYAADMDGTGDSVAH..GQFAPSR
M.vaccae	1MSSTDEPGAESGDATARARQ
M.vanbaalenii	1MRGRFPRRGGVSVSRQSLWPYAAGMASTDEPGVSGDPTARARQ
M.fortuitum	1MVSSN.PG.....H
M.smegmatis	1MASS.....
M.hassiacum	1MAGTDDVIGP..HSTRPQSR
M.tusciae	1MAGIDDVIG..GAAPQSR
M.neoaurum	1MASTDD.....A
M.rhodesiae	1MATTEDESGQ.....FEASR

M.tuberculosis	10	GESLWAHAEGSISEDEVILAGANERATDICGAVTPAYGALLCLLAKLSGGKAVAEVGTGA
M.bovis	10	GESLWAHAEGSISEDEVILAGANERATDICGAVTPAYGALLCLLAKLSGGKAVAEVGTGA
M.canettii	10	GESLWAHAEGSISEDEVILAGANERATDICGAVTPAYGALLCLLAKLSGGKAVAEVGTGA
M.marinum	43	AELLSAHAEGSISEDTILKTAANDRAVDICGAVTPAYGALLSMLAKLSGGKAVAEVGTGA
M.liflandii	43	AELLSAHAEGSISEDTILKTAANDRTVDICGAVTPAYGALLSMLAKLSGGKAVAEVGTGA
M.ulcerans	19	AELLSAHAEGSISEDTILKTAANDRAVDICGAVTPAYGALLSMLAKLSGGKAVAEVGTGA
M.triplex	22	AEALTTAHAEGSISEDAILGAMERSVDICGAVTPAYGALLSLLTKLSGGKAVAEVGTGA
M.genavense	16	ADALLAHAEGSISEDAILGAMERSVDICGAVTPAYGALLSLLTKLSGGKAVAEVGTGA
M.leprae	19	ADSLFAHAEGSISEDAILGAMERSVEICGAVTPAYGALLSLLTKLSGGKAVAEVGTGA
M.avium	17	AESLVAHAEGSISEDALLAANERAVDICGAVTPAYGALLSLLTKLSGGKAVAEVGTGA
M.colombiense	17	ADSLFAHAEGSISEDALLAANERAVDICGAVTPAYGALLSLLTKLSGGKAVAEVGTGA
M.kansasii	59	AELMSAHAEGSISEDAILGAMERAMDICGAVTPAYGALLSLLAKLSGGKAVAEVGTGA
M.vaccae	21	AAAIVNAHAEGSISEDAIVAAANERAVDICGAVTPAYGALLCVLAKVTGARAVVEVGTGA
M.vanbaalenii	47	AAAIVNAHAEGSISEDAIVAAANERAVDICGAVTPAYGALLCVLAKVTGARAVVEVGTGA
M.fortuitum	9	AAAIVTNAHAEGSISEDAIVAAANERAEICGAVTPAYGALLSVLARLTGARAVVEVGTGA
M.smegmatis	5	AAAIVTNAHAEGSISEDAIVAAANERADDICGAVTPAYGALLSVLARLTGARAVVEVGTGA
M.hassiacum	19	AAAIVAHAEGSISEDAIVAAANERAIDICGAVTPAYGALLCVLAKVTGARAVVEVGTGA
M.tusciae	17	AAAIVNAHAEGSISEDAIVAAANERAIDICGAVTPAYGALLCVLAKVTGARAVVEVGTGA
M.neoaurum	8	AQSIVNAHAEGSISEDAIVAAANERAVDSCGAVTPAYGALLSVLARLTGARAVVEVGTGA
M.rhodesiae	16	ADRILNAHAEGSISEDAIVAAANERAVDSCGAVTPAYGALLSVLARLTGARAVVEVGTGA

M.tuberculosis	70	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.bovis	70	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.canettii	70	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.marinum	103	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.liflandii	103	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.ulcerans	79	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.triplex	82	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.genavense	76	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.leprae	79	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.avium	77	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.colombiense	77	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.kansasii	119	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.vaccae	81	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.vanbaalenii	107	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.fortuitum	69	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.smegmatis	65	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.hassiacum	79	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.tusciae	77	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.neoaurum	68	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD
M.rhodesiae	76	GVSGLWLLSGMREDDGVLTTIDIEPEHLRLARQAFEAEGICPSRTRLISGRAOEVLTRLAD

M.tuberculosis	130	AS YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.bovis	130	AS YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.canettii	130	AS YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.marinum	163	DS YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.liflandii	163	DS YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.ulcerans	139	DS YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.triplex	142	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.genavense	136	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.leprae	139	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.avium	137	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.colombiense	137	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.kansasii	179	EAYDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.vaccae	141	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.vanbaalenii	167	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.fortuitum	129	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.smegmatis	125	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.hassiacum	139	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.tusciae	137	DS YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.neoaurum	128	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA
M.rhodesiae	136	ES YDLVFDADFDIDQPDVYEGVRLLRSGGIVVHRAALGSRAGDPGANDAEVIAVREAA

<i>M.tuberculosis</i>	190	<u>RLIAEDERLTPALVPLGDGVLAAVRD</u>
<i>M.bovis</i>	
<i>M.canettii</i>	190	RLIAEDERLTPALVPLGDGVLAAVRE
<i>M.marinum</i>	223	RLIAEDERLTPALVPLGDGVLAAVRD
<i>M.liflandii</i>	223	RLIAEDERLTPALVPLGDGVLAAVRD
<i>M.ulcerans</i>	199	RLIAEDERLTPALVPLGDGVLAAVRD
<i>M.triplex</i>	202	RLIAEDERLTPALVPLGDGVLAAVRD
<i>M.genavense</i>	196	RLIAEDERLTPAMVPLGDGVLAAVRD
<i>M.leprae</i>	199	RLIAENERLTPALVPLGDGLLAAVRE
<i>M.avium</i>	197	RLIAEDERLTPALVPLGDGILAAVRD
<i>M.colombiense</i>	197	RLIAEDERLTPALVPLGDGILAAVRD
<i>M.kansasii</i>	239	RLIAEDERLTPALVPLGDGLLAAVRE
<i>M.vaccae</i>	201	RLIAEDERLTPVLIPLGDGLLAAARD
<i>M.vanbaalenii</i>	227	RLIAEDDRLTPVLIPLGDGLLAAARD
<i>M.fortuitum</i>	189	RLIAEDERLTPVLIPLGDGLLAAARD
<i>M.smegmatis</i>	185	RLIAEDERLTPVLIPLGDGLLAAVRE
<i>M.hassiacum</i>	199	RLIAEDERLTPVLIPLGDGLLAAARD	FAAE
<i>M.tusciae</i>	197	RLIAEDERLTPVLIPLGDGLLAAARD
<i>M.neoaurum</i>	188	RLIAEDERFTPVLVPLGDGLLAAARD
<i>M.rhodesiae</i>	196	<u>RLIAEDERLTPVLIPLGDGILVAARD</u>	Y...

Figure S2 Alignment of primary sequences of homologues of *Mtb*OMT (Rv1220c) from different species of *Mycobacterium*. Interestingly, the His-Asp pair comprising of Asp138 and His164 is absolutely conserved in all species of *Mycobacterium*. Strictly conserved residues are highlighted with a red background.

M.tuberculosis
 Amycolicicoccus
 Nocardia
 Pilimelia
 Smaragdicoccus
 Rhodococcus
 Williamsia
 Microbispora
 Gordonia
 Actinomyces
 Arabidopsis 1 MSTG...LALNRCVSVVCRTAVTLNLR...PTVSVARSLKFSRRLLGNC
 Theobroma 1 MATG...FAISRCALAYQRAVVYLSRRQQFHALSSLTAKSRFLKLN. LTRNC
 Vitis 1 MACS...TAVN.HSVLGLQRQIVGKRLS...LLSLPAITNLGGIPRRRSCH
 Vanilla 1 MSASPWCLLPFFLSKPLFPPLPPTALGFVVKLPQLCVPSLRFLPFAMPFRYNDV
 Zea 1 MSSHLAAAASALPLPLPPPAVAAPSRALRALILSRGG.AAAVCSLRRGGTPACLVRRLC
 Rattus 1 MALPVPRLSIPALALGSAALG
 Homo 1 .GS

M.tuberculosis 1 .MPGQPAPSRGE...SLWAHAEGS.TSEKDVILAGANERATDLG..
 Amycolicicoccus 1 .MLANAD...LMLSHAESS.TIKDDILRAVNERADDLG..
 Nocardia 1 .RNLAYVEES.VVEDEILVSRNERATELG..
 Pilimelia 1 .MAVANVE...RNLAYVEES.VVEDEVLDSNERATELG..
 Smaragdicoccus 1 .MVAIAN...CTLSYVEES.VVEDDVVAARERAVDLG..
 Rhodococcus 1 .MLTNAE...RILTHTEDT.ILEDEMLATANDRAVELG..
 Williamsia 1 .MDPA...VLSRYAES.A.IVEDEALRLANERSDELG..
 Microbispora 1 .MDPA...VLSRYAEAA.IVEDEALRLANERSDELG..
 Gordonia 1 .MSDTAAAA...SLSEYAEAA.IIEDEALIEERMAEELG..
 Actinomyces 1 .MQEPLIYLLKPDFTKKVAEMNEKT...LSWSYCEDF.IPEGEVLETARQHARDFG..
 Arabidopsis 44 SIAPADPFYVADDKYGKQVVISLTP...RLYDYVLSN.VREPKILRQLREBETSKMRGS
 Theobroma 51 SSSSNAPFIVAEDKYGKQVVISITP...RLYDYILAN.VREPKILRQLREBETAMMRGS
 Vitis 46 VYAHLQPSVSDDFKYGKQVITITP...RLYDYILT.N.VREPKILRQLREBETAMMRGS
 Vanilla 56 NQAASVAVVTSEDERYKQVVISLTP...QLYDYVLAN.VREPKVLRQLREBETSVMRGS
 Zea 60 SHHSAATAALEARRGRKQGMTP...ALYDYLLAN.VREHPILRQLREBETAMMRGS
 Rattus 23 AAFATGLFLGKRFPWPYRRHQRLPQDNFLWQYLLSRSRREHPALRSLALLLLEQVQG
 Homo 3 .PPWRGRREQCQLPPEDSR.LWQYLLSRSRREHPALRSLALLLLEQVQG

M.tuberculosis 39 AGAVTFAVGALCLLAKLSGGKAVAEVGTGACVSGLWLLSGMRDDGVLTITIDIEPEHLRL
 Amycolicicoccus 34 ARAVTFAIGATLALLARLSDARAVVEIGTGACVSGLCMLMRGMRADGILITITIDTEHLRA
 Nocardia 34 AAFVPSVVGALLSMYQQLGARA VVEVGTGACVSGLWLLDGMREDGTLITIDSEPEHQRA
 Pilimelia 36 AAFVPSVVGALLSMYQQLGARA VVEVGTGACVSGLWLLDGMREDGTLITIDSEPEHQRA
 Smaragdicoccus 34 AAFVPSVVGALLSLFAQITGAKNVEVGTGACVSGLWLLDGMREDGTLITIDSEPEHQRA
 Rhodococcus 34 AAFVPSVVGALLSLFAQITGAKNVEVGTGACVSGLWLLDGMREDGTLITIDSEPEHQRA
 Williamsia 32 AFAITFAVGATLSLLARLVDAKAVVEVGTGACVSGLWLLNGMRTDGVLTITIDAEAEYHRA
 Microbispora 32 AFAITFAVGATLSLLARLVDAKAVVEVGTGACVSGLWLLNGMRTDGVLTITIDAEAEYHRA
 Gordonia 37 ATAISEATGALLSLLARLVDSHVEVIGTGACVSGLWLLAGMPENGLVLTITIDPEPEHRA
 Actinomyces 53 INTITSGVGAARMIVASCGARAVVEIGTGACVSGLWLLSGMSADAVLITIDIEPEHKKI
 Arabidopsis 99 QMQVSEDDQAQLLAMLVQILGARRCIEVGVYTCYSSLAVALALPESGCLVACERDARSLEV
 Theobroma 106 QMQVSEDDQAQLLAMLVQILGARRCIEVGVYTCYSSLAVALALPESGCLVACERDARSLEV
 Vitis 101 QMQVSEDDQAQLLAMLVQILGARRCIEVGVYTCYSSLAVALALPESGCLVACERDARSLEV
 Vanilla 111 QMLVSEDDQAQLLAMLVQILGARRCIEVGVYTCYSSLAVALALPESGCLVACERDARSLEV
 Zea 115 QMQVSEDDQAQLLAMLVQILGARRCIEVGVYTCYSSLAVALALPESGCLVACERDARSLEV
 Rattus 83 DSMMTCEQAQLLAMLARLIKAKRALDLEFTCYSSALALALALPEAGRVVTCSEVDAEPPKL
 Homo 50 DSMMTCEQAQLLAMLARLIKAKRALDLEFTCYSSALALALALPADGRVVTCEVDAQPEL

M.tuberculosis 99 ARQAFAEAGIGPSRTRLLISGRQEVLTRLA...DASYDLVFDADDPIDQPDVVAEGVRL
 Amycolicicoccus 94 ARRAFQEAAGIASTRTRLLINGRALDVLPRLA...DASYDLVFDANVVDQPPVVAASVRL
 Nocardia 94 AKEAFRAADIPPARTRLLINGRALDVLPRLA...DGAYDLVFDAAAPLEHPEYVAQGVRL
 Pilimelia 96 AKEAFRTAEIPPARTRLLINGRALDVLPRLA...DGAYDLVFDAAAPMEHPFYVEQGVRL
 Smaragdicoccus 94 AREAFRAGGVAPSRTRLLINGRALDVLPRLQ...DGNVYDLVFDADDPVYPTVYVEQAVRL
 Rhodococcus 94 AKQTFRVAQVAPSRTRLLINGRALDVLPRLA...DASYDLVFDANAPADHPHFVREGVRL
 Williamsia 92 ARLAFTTAGIIPSRTRLLINGRAAEVLPRLA...DASYDLVFDGAVTDQPRVVAEGLRL
 Microbispora 92 ARLAFTTAGIIPSRTRLLINGRAAEVLPRLA...DASYDLVFDGAVTDQPRVVAEGLRL
 Gordonia 97 ARETFADAHIGPSRTRLLINGRALTDLTRLA...DETYDLVFDGAPLSYPLFVTEHTRI
 Actinomyces 113 ARTAFAAAGMRPPTRLITGQALDILPRMA...ARAYDLVFDADDPQMHAYIAEATRM
 Arabidopsis 159 AKRYNELAGVS.HKVVVKHGLAASDLKSMIQNGEGASVDFAFVDAKRMVQDYFELLQL
 Theobroma 166 AKKYNELAGVS.HKVVVKHGLAASDLKSMILNGEACSYDFAFVDAEKRMQEFYFELLQL
 Vitis 161 AKRYNELAGVS.HKVVVKHGLAASDLKSLNGEESVDFAFVDAEKRMQEFYFELLQL
 Vanilla 171 AKKYNRAAGVS.HKVEIRHGLAYDTLVHLEIRGKSCSDFAFVDAKIKYGEYYELLQL
 Zea 175 AKKYNRAAGVA.HKVIDVKHGLAASDLRSLLDCGEASVDFAFVDAEKRMVYEEYELLKL
 Rattus 143 GRPLMRQAEVE.HKIDLRQLQFALDLELLAAGEAGTFDFAVVDAKENCATYIERCQL
 Homo 110 GRPLMRQAEVE.HKIDLRQLQFALDLELLAAGEAGTFDFAVVDAKENCATYIERCQL

M.tuberculosis 155 LRSGLVIVVHRAALGGRAGDGFARDAEVIAVREAAARLIAEDERLTPALVPLGDGVLAAVR
 Amycolicicoccus 150 LRFSGALVVNASMLGSRVGFDFSQDDAAALSREAAQLIADDETLTSVLIPLGEGGLLCAAR
 Nocardia 150 LRECGAILHNNALLGSRVGFDFQTDVAVTQAVSATRAIAEDERLTCVLIPLVGDGLLCAAR
 Pilimelia 152 LRECGAFILHNNALLGSRVGFDFQTDVAVTQAVSATRAIAENBELTSVLIPLGEGGLLCAAR
 Smaragdicoccus 150 LRFSGAMLLHNNALPGSLGDAQRDPTVAVTAATAIAEDERLTSVLIPLVGVGLMAAVR
 Rhodococcus 150 LRFSGVIVLHNNALLGSRVAFDFPDAATVAVREAAARIAADDERLTVLPLVGDGLLCAAR
 Williamsia 148 LRGGCILLIVHNASADGTVADEFSTDPAAQAREGALLIADDDTLPPVVIPLGRGLLAAAK
 Microbispora 148 LRGGCILLIVHNASADGTVADEFSTDPAAQAREGALLIADDDTLPPVVIPLGRGLLAAAK
 Gordonia 153 LRFSGLVVVNNASADGTVADEFSTDPAAQAREGALLIADDDTLPPVVIPLVGDGLLAAAK
 Actinomyces 169 LRSGVIVVVAHALWNDTVADEFARREPEFVAIEQLGKDLADSEDFMTITPLVGDGLLVAVR
 Arabidopsis 218 VRVSGVIVMDNVLWHGRVSDPMVNDAKTISIRNFNKKLMDDKRVVSISSMVEIGDGMTICRK
 Theobroma 225 VRVSGVIVMDNVLWHGRVADPLVNDAKTISIRNFNRRNVMEDKRVVSISSMVEIGDGMTICRK
 Vitis 220 VRTRGVIVIDNVLWHGRVADPLVNDARTVSIIRNFNKNIMEDKRVVSISSMVEIGDMITICRK
 Vanilla 230 VRVSGVIVMDNVLWHGRVSDPMVNDQKTISIRNFNKKRILEDKRVVSISSMVEIGDGMTICRK
 Zea 234 VRVSGVIVMDNVLWYGRVADPLVNDQKTISIRNFNKKVLEDKRVVSISSMVEIGDMITICRK
 Rattus 202 LRFSGVLAVLRVLRGSEVLPQPKMKAVECVRNLNERILRDRARVYISLLPLDDGLSLAFK
 Homo 169 LRFSGVLAVLRVLRGSKVLPQPKGDVAEECVRNLNERILRDRARVYISLLPLDDGLSLAFK

<i>M.tuberculosis</i>	215	D.....
<i>Amycolobicoccus</i>	210	K.....
<i>Nocardia</i>	210	G.....
<i>Pilimelia</i>	212	C.....
<i>Smaragdicoccus</i>	209	R.....
<i>Rhodococcus</i>	210	L.....
<i>Williamsia</i>	208	ARTDLG.
<i>Microbispora</i>	208	ARTDLG.
<i>Gordonia</i>	213	A.....
<i>Actinomyces</i>	229	R.....
<i>Arabidopsis</i>	278	R.....
<i>Theobroma</i>	285	R.....
<i>Vitis</i>	280	R.....
<i>Vanilla</i>	290	RETDQSL
<i>Zea</i>	294	LVDT...
<i>Rattus</i>	262	I.....
<i>Homo</i>	229	I.....

Figure S3 Alignment of primary sequences of homologues of *Mtb*OMT (Rv1220c). His-Asp pair comprising of Asp138 and His164 is conserved in some microbial genus. Strictly conserved residues are highlighted with a red background. Conserved residues are marked in red.

Table S1 Metal ion analysis of *Mtb*OMT by ICP-AES.

Metal ion (characteristic spectrum / nm)	Ca²⁺ (317.93)	Zn²⁺ (213.85)	Mg²⁺ (279.55)	Mn²⁺ (260.57)
Blank (detection limit / ppm)	0.0069	0.0012	0.0009	0.0009
Blank / ppm (RSD in %)	0.2153 (1.058)	0.0126 (2.818)	0.0515 (0.5337)	0.0024 (2.761)
Sample / ppm (RSD in %)	0.2338 (0.4004)	0.0229 (0.6503)	0.0569 (0.1619)	0.0038 (1.779)
Sample - Blank / ppm	0.0185	0.0103	0.0054	0.0014

S1. Inductively coupled plasma atomic emission spectroscopy (ICP-AES)

Buffer (20mM HEPES, pH7.5, 100mM NaCl) was used as the blank control. Purified *Mtb*OMT was buffer exchanged into blank buffer. Both blank buffer and protein sample were digested with 5% v/v nitric acid. Then the samples were analysed using an ICP-AES Thermo Scientific iCAP IRIS Advantage instrument. In total 4 elements, *i.e.* Ca²⁺, Zn²⁺, Mg²⁺, and Mn²⁺, were analysed (Supplementary Table 1).