

Title of the manuscript:

Modeling Permeability of Drug-like Molecules through Mycobacterium Tuberculosis Cell Wall: An Analogue Based Approach” by Sridhara Janardhan, M. Ram Vivek and G. Narahari Sastry

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Description about the script

Five QSAR models have been developed based the differential activity between enzyme based assays and cell-based assays. Hence, we have written a shell script based on these five models for the prediction and prioritization of unknown compounds. The script follows the following steps

1. Calculate PaDEL descriptors for the user given input sdf molecules.
2. Calculated PaDEL descriptors for the input molecules are saved as ouput.csv format with comma separated
3. The header in outout.csv is separated and saved as noheader.csv
4. Identifies the molecular descriptors obtained from the QSAR models (a total of 68 descriptors for five models)
5. Each descriptor header is mapped with the corresponding descriptor values calculated from PaDEL
6. Define the descriptor coefficients for each model along with the intercept value
7. Each calculated descriptor value is multiplied with the corresponding descriptor coefficient followed by addition of intercept.
8. This process continued iteratively for all the molecules and for all the models.
9. The predictive values for all the models are displayed as an output

Script:

```
#!/bin/sh
Java -jar ~/PaDEL-Descriptor.jar -2d -dir input.sdf -file output.csv
cat output.csv | sed "1 d" > noheader.csv
file=output.csv
separator=","
column="ALogp2"
column1="ATSC1e"
column2="ATSC5i"
column3="AATSC2c"
column4="AATSC3p"
column5="MATS7i"
column6="MATS1s"
column7="GATS6s"
column8="VR2_Dzp"
column9="SM1_Dzs"
column10="SC-5"
column11="nHBint3"
column12="mindsN"
column13="ETA_Epsilon_3"
column14="MDEC-22"
column15="AATS2i"
column16="AATSC3e"
column17="AATSC3i"
column18="GATS6e"
column19="GATS1s"
column20="GATS8s"
column21="VR1_Dzp"
column22="SM1_Dzs"
column23="VCH-5"
column24="VE2_Dt"
column25="nHsOH"
column26="minHssNH"
column27="maxsssCH"
column28="maxssO"
column29="ETA_Psi_1"
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column30="nHBacc_Lipinski"
column31="nFRing"
column32="ATSC3i"
column33="AATSC5c"
column34="MATS1m"
column35="MATS2e"
column36="GATS6m"
column37="BCUTp-11"
column38="SpMin1"
column39="SHBd"
column40="mindsN"
column41="maxHBint2"
column42="R_TpiPCTPC"
column43="SRW9"
column44="AATSC6c"
column45="GATS7c"
column46="SpMAD"
column47="BCUTc-11"
column48="SpMin1"
column49="C3SP2"
column50="SHBd"
column51="minHdsCH"
column52="mindsN"
column53="maxHBint2"
column54="sumI"
column55="piPC10"
column56="topoShape"
column57="AATSC5e"
column58="GATS8c"
column59="BCUTc-11"
column60="SpMin1"
column61="C3SP2"
column62="minHBint2"
column63="minHsOH"
column64="mindsN"
column65="MDEN-22"
column66="R_TpiPCTPC"
column67="topoShape"
for column_name in $(head -n 1 $file | tr $separator " ");
do
  [[ $column_name == $column ]] && break
  field=$((field+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
  [[ $column_name == $column1 ]] && break
  field1=$((field1+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
  [[ $column_name == $column2 ]] && break
  field2=$((field2+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
  [[ $column_name == $column3 ]] && break
  field3=$((field3+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
  [[ $column_name == $column4 ]] && break
  field4=$((field4+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
  [[ $column_name == $column5 ]] && break
  field5=$((field5+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do

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[[ $column_name == $column6 ]] && break
field6=$((field6+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column7 ]] && break
field7=$((field7+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column8 ]] && break
field8=$((field8+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column9 ]] && break
field9=$((field9+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column10 ]] && break
field10=$((field10+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column11 ]] && break
field11=$((field11+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column12 ]] && break
field12=$((field12+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column13 ]] && break
field13=$((field13+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column14 ]] && break
field14=$((field14+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column15 ]] && break
field15=$((field15+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column16 ]] && break
field16=$((field16+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column17 ]] && break
field17=$((field17+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column18 ]] && break
field18=$((field18+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column19 ]] && break
field19=$((field19+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
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[[ $column_name == $column20 ]] && break
field20=$((field20+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column21 ]] && break
field21=$((field21+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column22 ]] && break
field22=$((field22+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column23 ]] && break
field23=$((field23+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column24 ]] && break
field24=$((field24+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column25 ]] && break
field25=$((field25+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column26 ]] && break
field26=$((field26+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column27 ]] && break
field27=$((field27+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column28 ]] && break
field28=$((field28+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column29 ]] && break
field29=$((field29+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column30 ]] && break
field30=$((field30+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column31 ]] && break
field31=$((field31+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column ]] && break
field32=$((field32+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column32 ]] && break
field32=$((field32+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do

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[[ $column_name == $column33 ]] && break
field33=$((field33+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column34 ]] && break
field34=$((field34+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column35 ]] && break
field35=$((field35+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column36 ]] && break
field36=$((field36+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column37 ]] && break
field37=$((field37+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column38 ]] && break
field38=$((field38+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column39 ]] && break
field39=$((field39+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column40 ]] && break
field40=$((field40+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column41 ]] && break
field41=$((field41+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column42 ]] && break
field42=$((field42+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column43 ]] && break
field43=$((field43+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column44 ]] && break
field44=$((field44+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column45 ]] && break
field45=$((field45+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column46 ]] && break
field46=$((field46+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
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[[ $column_name == $column47 ]] && break
field47=$((field47+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column48 ]] && break
field48=$((field48+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column49 ]] && break
field49=$((field49+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column50 ]] && break
field50=$((field50+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column51 ]] && break
field51=$((field51+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column52 ]] && break
field52=$((field52+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column53 ]] && break
field53=$((field53+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column54 ]] && break
field54=$((field54+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column55 ]] && break
field55=$((field55+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column56 ]] && break
field56=$((field56+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column57 ]] && break
field57=$((field57+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column58 ]] && break
field58=$((field58+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column59 ]] && break
field59=$((field59+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column60 ]] && break
field60=$((field60+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
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[[ $column_name == $column61 ]] && break
field61=$((field61+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column62 ]] && break
field62=$((field62+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column63 ]] && break
field63=$((field63+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column64 ]] && break
field64=$((field64+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column65 ]] && break
field65=$((field65+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column66 ]] && break
field66=$((field66+1))
done
for column_name in $(head -n 1 $file | tr $separator " ");
do
[[ $column_name == $column67 ]] && break
field67=$((field67+1))
done
field=$((field+1))
field1=$((field1+1))
field2=$((field2+1))
field3=$((field3+1))
field4=$((field4+1))
field5=$((field5+1))
field6=$((field6+1))
field7=$((field7+1))
field8=$((field8+1))
field9=$((field9+1))
field10=$((field10+1))
field11=$((field11+1))
field12=$((field12+1))
field13=$((field13+1))
field14=$((field14+1))
field15=$((field15+1))
field16=$((field16+1))
field17=$((field17+1))
field18=$((field18+1))
field19=$((field19+1))
field20=$((field20+1))
field21=$((field21+1))
field22=$((field22+1))
field23=$((field23+1))
field24=$((field24+1))
field25=$((field25+1))
field26=$((field26+1))
field27=$((field27+1))
field28=$((field28+1))
field29=$((field29+1))
field30=$((field30+1))
field31=$((field31+1))
field32=$((field32+1))
field33=$((field33+1))
field34=$((field34+1))
field35=$((field35+1))
field36=$((field36+1))
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field37=$((field37+1))
field38=$((field38+1))
field39=$((field39+1))
field40=$((field40+1))
field41=$((field41+1))
field42=$((field42+1))
field43=$((field43+1))
field44=$((field44+1))
field45=$((field45+1))
field46=$((field46+1))
field47=$((field47+1))
field48=$((field48+1))
field49=$((field49+1))
field50=$((field50+1))
field51=$((field51+1))
field52=$((field52+1))
field53=$((field53+1))
field54=$((field54+1))
field55=$((field55+1))
field56=$((field56+1))
field57=$((field57+1))
field58=$((field58+1))
field59=$((field59+1))
field60=$((field60+1))
field61=$((field61+1))
field62=$((field62+1))
field63=$((field63+1))
field64=$((field64+1))
field65=$((field65+1))
field66=$((field66+1))
field67=$((field67+1))
echo $field
echo $field1
echo $field2
echo $field3
echo $field4
echo $field5
echo $field6
echo $field7
echo $field8
echo $field9
echo $field10
echo $field11
echo $field12
echo $field13
echo $field14
echo $field15
echo $field16
echo $field17
echo $field18
echo $field19
echo $field20
echo $field21
echo $field22
echo $field23
echo $field24
echo $field25
echo $field26
echo $field27
echo $field28
echo $field29
echo $field30
echo $field31
echo $field32
echo $field33
echo $field34
echo $field35
echo $field36
echo $field37
echo $field38
```



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echo $field39
echo $field40
echo $field41
echo $field42
echo $field43
echo $field44
echo $field45
echo $field46
echo $field47
echo $field48
echo $field49
echo $field50
echo $field51
echo $field52
echo $field53
echo $field54
echo $field55
echo $field56
echo $field57
echo $field58
echo $field59
echo $field60
echo $field61
echo $field62
echo $field63
echo $field64
echo $field65
echo $field66
echo $field67
while [ $loop -ne 0 ]
do
a1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field}')
b1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field1}')
c1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field2}')
d1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field3}')
e1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field4}')
f1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field5}')
g1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field6}')
h1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field7}')
i1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field8}')
j1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field9}')
k1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field10}')
l1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field11}')
m1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field12}')
n1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field13}')
o1=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field14}')
a2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field15}')
b2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field16}')
c2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field17}')
d2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field18}')
e2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field19}')
f2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field20}')
g2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field21}')
h2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field22}')
i2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field23}')
j2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field24}')
k2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field25}')
l2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field26}')
m2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field27}')
n2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field28}')
o2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field29}')
p2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field30}')
q2=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field31}')
a3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field32}')
b3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field33}')
c3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field34}')
d3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field35}')
e3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field36}')
f3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field37}')
g3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $field38}')

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h3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field39}')
i3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field40}')
j3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field41}')
k3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field42}')
l3=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field43}')
a4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field44}')
b4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field45}')
c4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field46}')
d4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field47}')
e4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field48}')
f4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field49}')
g4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field50}')
h4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field51}')
i4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field52}')
j4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field53}')
k4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field54}')
l4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field55}')
m4=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field56}')
a5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field57}')
b5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field58}')
c5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field59}')
d5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field60}')
e5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field61}')
f5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field62}')
g5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field63}')
h5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field64}')
i5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field65}')
j5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field66}')
k5=$(awk 'FNR == $inc' noheader.csv | awk -F, '{print $$field67}')
a1z=0.0429
b1z=0.8048
c1z=-0.0129
d1z=-252.2425
e1z=3.6993
f1z=1.3191
g1z=-5.5064
h1z=0.7633
i1z=0.0173
j1z=0.4744
k1z=-0.7232
l1z=-0.3949
m1z=0.3272
n1z=-51.4922
o1z=0.0221
a2z=-0.0809
b2z=48.3046
c2z=1.9709
d2z=0.4669
e2z=2.7181
f2z=-0.7886
g2z=0.0011
h2z=0.2564
i2z=3.7615
j2z=66.9653
k2z=-1.1684
l2z=-1.4188
m2z=-1.0973
n2z=-0.0498
o2z=-18.9726
p2z=0.1130
q2z=-0.1447
a3z=0.0073
b3z=-92.3317
c3z=-8.155
d3z=-0.988
e3z=-0.3572
f3z=-0.4748
g3z=4.1623
h3z=-1.4682
i3z=0.3973
```

```

j3z=0.172
k3z=-0.3275
l3z=-0.0812
a4z=99.9479
b4z=-1.1737
c4z=-0.1649
d4z=-6.3326
e4z=4.8634
f4z=-0.2189
g4z=-1.4585
h4z=-2.3849
i4z=0.2553
j4z=0.1914
k4z=0.0309
l4z=-0.3473
m4z=3.5827
a5z=-10.6561
b5z=-0.7539
c5z=-6.8146
d5z=8.4696
e5z=-0.2556
f5z=0.1043
g5z=-1.9977
h5z=0.3545
i5z=-0.7255
j5z=-0.2836
k5z=3.375
for
do
Model1=$(echo "$a1 * $a1z + $b1 * $b1z + $c1 * $c1z + $d1 * $d1z + $e1 * $e1z + $f1 * $f1z + $g1 * $g1z + $h1 * $h1z + $i1 * $i1z + $j1 * $j1z + $k1 * $k1z + $l1 * $l1z + $m1 * $m1z + $n1 * $n1z + $o1 * $o1z + 25.1491" | bc)
echo $Model1
inc=$(echo "$inc +1" | bc)
loop=$(echo "$loop -1" | bc) && break
done
for
do
Model2=$(echo "$a2 * $a2z + $b2 * $b2z + $c2 * $c2z + $d2 * $d2z + $e2 * $e2z + $f2 * $f2z + $g2 * $g2z + $h2 * $h2z + $i2 * $i2z + $j2 * $j2z + $k2 * $k2z + $l2 * $l2z + $m2 * $m2z + $n2 * $n2z + $o2 * $o2z + $p2 * $p2z + $q2 * $q2z + 26.121" | bc)
echo $Model2
inc=$(echo "$inc +1" | bc)
loop=$(echo "$loop -1" | bc) && break
done
for
do
Model3=$(echo "$a3 * $a3z + $b3 * $b3z + $c3 * $c3z + $d3 * $d3z + $e3 * $e3z + $f3 * $f3z + $g3 * $g3z + $h3 * $h3z + $i3 * $i3z + $j3 * $j3z + $k3 * $k3z + $l3 * $l3z + 2.2595" | bc)
echo $Model3
inc=$(echo "$inc +1" | bc)
loop=$(echo "$loop -1" | bc) && break
done
for
do
Model4=$(echo "$a4 * $a4z + $b4 * $b4z + $c4 * $c4z + $d4 * $d4z + $e4 * $e4z + $f4 * $f4z + $g4 * $g4z + $h4 * $h4z + $i4 * $i4z + $j4 * $j4z + $k4 * $k4z + $l4 * $l4z + $m4 * $m4z -3.9556" | bc)
echo $Model4
inc=$(echo "$inc +1" | bc)
loop=$(echo "$loop -1" | bc) && break
done
for
do
Model5=$(echo "$a5 * $a5z + $b5 * $b5z + $c5 * $c5z + $d5 * $d5z + $e5 * $e5z + $f5 * $f5z + $g5 * $g5z + $h5 * $h5z + $i5 * $i5z + $j5 * $j5z + $k5 * $k5z -13.7677" | bc)
echo $Model5
inc=$(echo "$inc +1" | bc)
loop=$(echo "$loop -1" | bc) && break
done

```
