



Computational Chemical Biology and

-. / \$01002

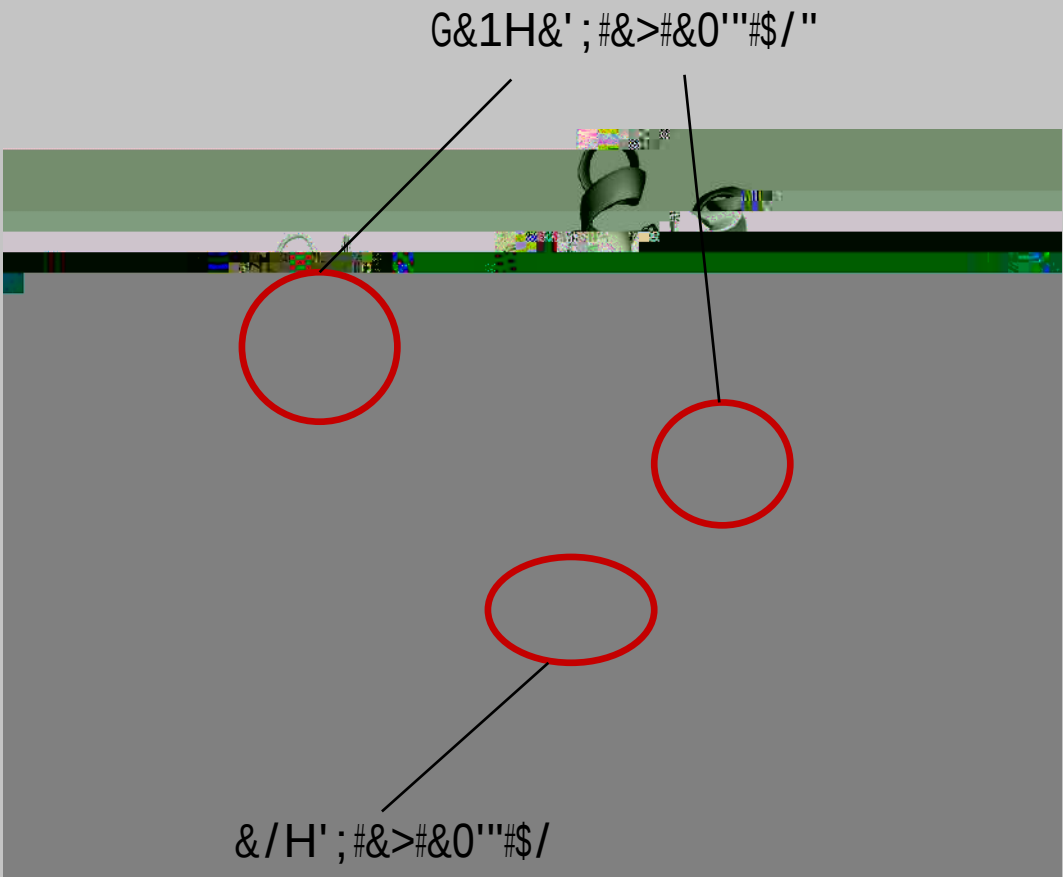
&33454"&647\$5+,&' 78 / &99+' , \$ / .543:5&"\$7; ' & / +3<\$=&> ? ? !@\$746436<\$3";96+3\$A+' 7+' , \$<+64<



B995;+ ' , \$&> ? ? ! \$6 . \$&\$7" : , \$6&" , 46



EF+%&>/> *)9+\$#* +1*G/\$ +)/>#*\$> ;9 %@ 6 6 8
%&> .%,#>%\$> ;9 &/H I=)%9 *)9"\$%, "\$)4*\$4)/"



%@ 6 6 8 +)/>#*\$> \$7/ \$H1 G&1H& ;#&>#&0 "'#\$/"
%&> % &/H ;#&>#&0 "'#\$/



4 5 6 7 6 (" >?(@6' ("

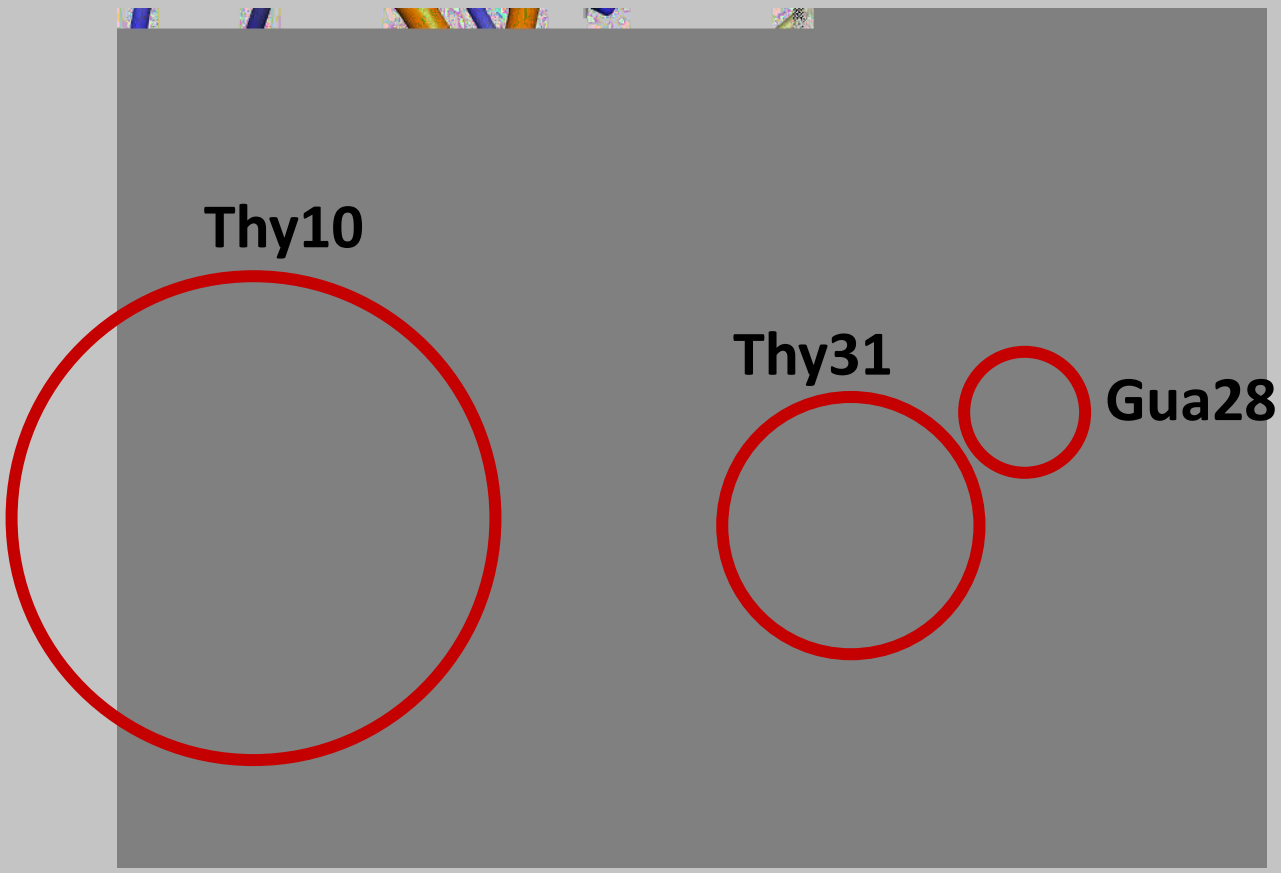
J4&>/>' ;9'5K8L'()/=(# ,1\$

*6":36:"48A&<47\$74<+, '\$.C\$! DB\$&96& / 4"<

- ▶ !+\$% 3 /)""%) /""#&0, /="\$)%&> />'8M!'1)'LM!' 3 1, / *4, /""H#\$7'4&#N4 / '\$ /)\$#%)9""\$)4*\$4) /"
- ▶ K7 /9'7%. /', # 3 #\$/>' *7 / 3 #*%, '>#. /)'#\$9'; / *%4" / '\$7 /) /'%) /'1&, 9'O'&%\$4)% , '&4*, / 1\$#> /""%. %#, %; , /'P1)"" / , / *\$#1&
- ▶ Q&&%\$4)% , '&4*, / 1\$#> /"" *14, >'#&*) / %" / '\$7 /'P4& *\$#1&%, #9'1P'%+\$% 3 /)"" ; 9'+)1.#>#&0'%>>#\$1&%, '*7 / 3 #*%, '%&>' "\$)4*\$4)% , '>#. /)'#\$9'; /91&>'\$7%\$'+)1.#> />' ; 9'&%\$4)% , '&4*, / 1\$#> /"
- ▶ R /& /\$#*'% , +7% ; /\$' /F+%&> />'H#\$7'> / . / , 1+ 3 /&\$'1P'8"

> ? ? ! \$ < + / : 5 & 6 + . ' < \$ 7 4 ' 6 + C ; \$ 6 E " 4 4 \$ E ; 7 " . 9 E . A + 3 \$ A + ' 7 + ' , \$ < + 6 4 < \$ ' 4 & " \$ & 9 6 & / 4 " \$ A + ' 7 + ' , \$ + ' 6 4 " C & 3 4 \$) + 6 E \$ F G -

- ▶ . 1 & ' T # , , / ;) % & > ' P % * \$ 1) ' ? . T J A ' # " " % ' +) 1 \$ / # & ' P 1 4 & > ' # & ' ; , 1 1 > ' + , % " 3 % ' \$ 7 % \$ ' P % * # , # \$ % \$ / " " ; , 1 1 > ' * , 1 \$ \$ # & 0
- ▶ ! " " \$ 7 / ' 8 " " & 4 * , / 1 \$ # > / ' # " " 7 # 0 7 , 9 ' 7 9 >) 1 + 7 1 ; # * U ' ; / & D / & / " " H /) / ' 4 " / > ' # & ' @ 6 6 8 " " # 3 4 , % \$ # 1 & " " \$ 1 ' # > / & \$ # P 9 ' + 4 \$ % \$ # . / ' 8 " " # & \$ /) % * \$ # 1 & " " # \$ / " " 1 & ' ! V ' > 1 3 % # & ' 1 P ' . T J



! " # \$ " # " % & ' ' () * # ' + % , *) % & - % . / % 0 & , * 1 # % & - % 2 3 4

!<\$<:A<6+6:6+. '<\$&6\$9.<+6+. '<\$H1I\$OJ\$&' 7\$KH\$+'\$&96&/ 4"\$BLMHHNO

▶ 8""4;"#\$4\$#1&""+)/.#14",9'#\$)1>4*/>'\$1'!LWVVB'%\$'+1""\$#1&""VCU'BY'%&>'ZV

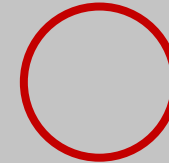
▶

? .543:5&"\$ / .7455+ ' ,\$.C\$! <8<:A<6+6:647\$BLMHHNO\$74"+F&6+F4<

!"#\$%&' (##) *

!"*+%&' (##) *

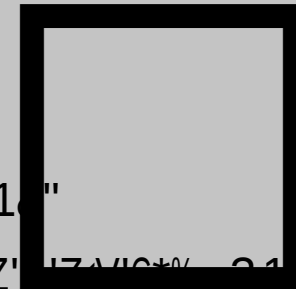
!",#%&' (##) *



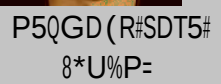
J 5%6#*)6E&86%6E&G1#F%
*>8"?#*812"% '&#-&? , *81%&-%
56/K

56<L% , &0">>"0%&% '?+68*>%
68? ('8(?"%=@ABC%DE1&)E"#"%"?1#F%
&-%56<L%0&"6%#&8%&2"?>*)%G18E%

56=/% , &0">>"0%&% '?+68*>%
68? ('8(?"%=@ABC%DE1&)E"#"%"?1#F%
&-%56=/%'>*6E"6%G18E%HE" / = I ; C



- ▶ 8"VC'%&>'8"BY'>/)#. %\$#. /'')/ 3 %&#&/>' ; 14&>'\$1'. T J'\$7)1407' 6 8'"# 3 4,%\$#1 " "
- ▶ 2#&>#&0'P)/ /' /&/)0#/'"%) /'&1\$'"#0&#P#*%&\$,9'>#PP)/&\$'P)1 3 ' ! LWVVXB'?=VYY<Z' 17140*% _ 2 1 A

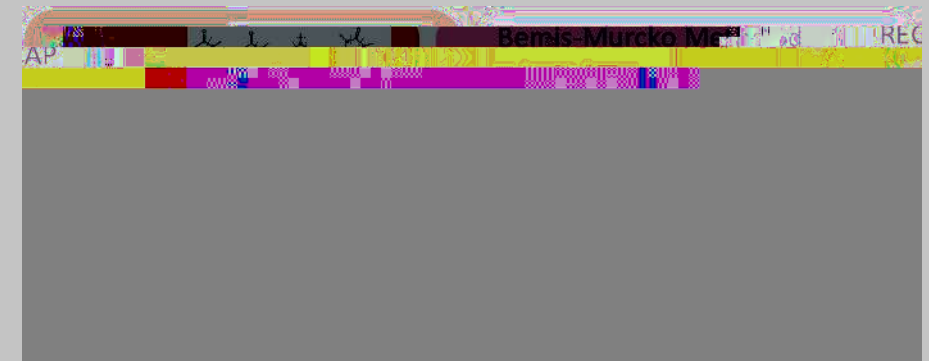
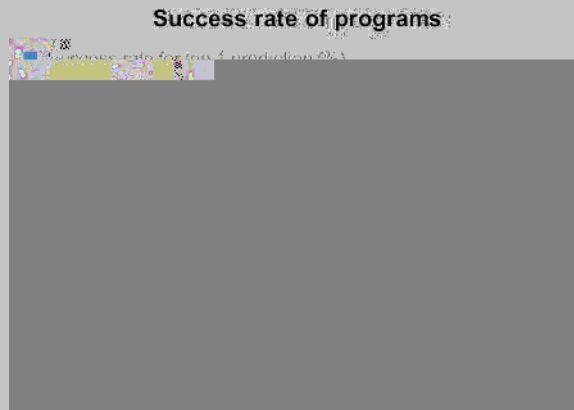


S55#P#5K# 'H# . /3(62/4%# . , - , , .#0M.#01LM301M,
; B' (#**)5K# 'H#V; *#WG5"'.# , - , , .#0.#0/MN130/MO-
: 5X6K'# : Y#5K# 'H#5\$/) & /2%, -126.# , - , L.#ON.#O-2

P '64" ' <Q\$"4<4&"3E

!"#\$%#&'()* (+*, -(&.')/012*3(45')6*7 .&8(39

!"#\$%#&'()* (+*3'++.-.)&*+-#6 7 .)&#&'()*
7 .&8(39*+(-*-#6 7 .)&*3#&#:#9.*,-.,#-#&'()



- ▶ H=5] : ^%68&))"0%G&?S1#F%E*>-G*+%8E?&(FE%8E"%)?&\ "'8%
*#0%6&%#(, 7"?%&-%8"68%'*6"6%G*6%6 , *>>
- ▶ . ' ' (?*' + _3(, -?)' %Y% @5] : ^%Y% `5] : ^%Y% =09H :
- ▶ V) ""0 _C@D3E%Y% @5] : ^%Y% : > (6H?&%a% =09H :

- F?G!FFD%G*6%8E"%7"68%-?*F , "#8*81&#% , "8E&0%*6%18%F"#"?*"8"6%
-?*F , "#86%8E*8_
- ▶ *?"%E1FE>+%(#1b("
 - ▶ -&>&G%8E"%c?(>"%&-%8E?" "d%8&%8E"%F?"*8"68%" [8"#8

:>*?*D*#Z% @*?!6E1F*%e>*#F&2*#%*#O%W1 , % f (%g1#F%MV9HU%

B3R' .) 547,4 / 4 '6<

; &#++<

`4"\$#&'M0

6 /&0'a7/&94

W71&0'b#%&'W7//

