1(:6/(77(5 6XPPHU

CHEMICAL INFORMATION & COMPUTER APPLICATIONS GROUP

OUTBREAK

&RQWULEXWHG E\ 'LDQD /HLWFK ,QIRUPDWLRQ &RQVXOWDQ

)ROORZLQJ RQ IURP VXFFHVV LQ WKH 56& ,<& &KDOOHQ
&,&$* 6SULQJ 1HZVOHWWHU JUDQW ZRQ E\ WKH 56& V W
+LVWRULFDO *URXS DQG &,&$* ZDV XVHG WR IXQG D QHZ
&DWDO\VW 6FLHQFH 'LVFRYHU\ &HQWUH :LQGHV

2XU%5($. ZDV ODXQFKHG RQ)HEUXDU\ &DWDO\VW ZDV HQJDJHG SRW

- 5XQFRUQ DQG :LQGHQVG:RUOWK)HEUXDU\ KWWSV ZZZ UXQFRUQDQGZLGQHVZRUOG FR XN QHZV VBBB B BWRBGHYHORSBH[FLWLQJBFKHPLVWU\BSURMH
- 56& 1HZVOHWWHU LVVXH SDJH KWWSV PDJ GLJLWDOSF FR XN IY[UVF UVFQ
- 6RO\D\ &RQVXOWDQF\ SDJH KWWSV ZZZ VRO\D\ FR XN HQ ELQDULHV 6RO\D\ &RQQH

&RQWDFW GDQD OHLWFK#JPDLO FRP
&DWDO\VW 6FLHQFH 'LVFRYHU\ &HQWUH XN

BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB

Student Bursaries

,Q RUGHU WR HQFRXUDJH \RXQJ FKHPLVWV WR FRQVLGHU
FRPSXWHU DSSOLFDWLRQV WKH &,&$* FRPPLWWHH LV SU
VWXGHQWV IRU EXUVDULHV WR DWWHQG DQ\ UHOHYDQW FK
FRQIHUHQFH RU PHHWLQJ
,QLWLDO HQTXLULHV VKRXOG EH PDGH WR WKH &,&$* &
KHOHQ FRRNH #JPDLO FRP

BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB

Sponsorship

7KLV \HDU &,&$* KDV DHOGWKDGHVHSYRQVRV

)LUVW MRLQW &,&$* &DPEULGJH &KHPLQIRUPDWLFV 1HWZ
7KLV PHHWLQJ WRRN SODFH RQ WKH DIWHUQRRQ RI :HGQH
&U\VWDOORJUDSKLF 'DWD &HQWUH &&'& LQ &DPEULGJH D
FDNH DQG FRIIHH WHD EHIRUH WKH PHHWLQJ 7KH SURJUDP

- 6HPDQWLF 5HSUHVHQWDWLRQ RI &KHPLFDO ,QIRUPDWL 0DUN %RUNXP 8QLYHUVLW\ RI 6RXWKDPSWRQ KWWSV XN OLQNHGLQ FRP SXE PDUN ERUNXP E E
-

5 6 & & , & $ * 1 H Z V O H W W H U 6 X P P H U

5 6 & & , & $ * 1 H Z V O H W W H U 6 X P P H U

- D PDMRU DQG RU VXVWDLQHG FRQWULEXWLRQ WR XQGHUVWDQGLQJ RI WKH LQIRUPDWLRQ UHWULHYDO SU
- GHYHORSPHQW RI RU VLJQLILFDQW LPSURYHPHQW LQ WKH UHWULHYDO RI LQIRUPDWLRQ HLWKHU JHQHUDOO
- GHYHORSPHQW RI RU VLJQLILFDQW LPSURYHPHQW L VHUYLFH
- GHYHORSPHQW DQG RU H[SORLWDWLRQ RI QHZ WHF UHWULHYDO
- D VXVWDLQHG FRQWULEXWLRQ RYHU D SHULRG RI \HD IRU H[DPSOH E\ UXQQLQJ DQ LQIRUPDWLRQ VHUYLFH LQWHUQDWLRQDO OHYHO WR RUJDQLVDWLRQV DFWLYH

.H\ FKDUDFWHULVWLFV WKDW WKH MXGJHV ZLOO ORRN IR RULJLQDOLW\ DQG SUDFWLFDOLW\

)XOO GHWDLOV RI KRZ WR DSSO\ FDQ EH IRXQG DW KWWS ZZZ XNHLJ RUJ XN FRQWHQW FDOO WRQ\ NHQW

3UHVHQWDWLRQ RI -DVRQ)DUUDGDQH DQG WKH 7RQ\ .H 2QFH DJDLQ ,QWHUQHW /LEUDULDQ ,QWHUQDWLRQDO SOD\H ZKLFK WRRN SODFH DW WKH EHJLQQLQJ RI WKH .H\QRWH QRPLQDWLRQV IRU ERWK WKH -DVRQ)DUUDGDQH DQG WKH ZLQQHUV ZHUH IRXQG IRU ERWK

7KH -DVRQ)DUUDGDQH $ZDUG ZHQW WR 3URIHVVRU &KI QRPLQDWLRQ VD\V LV VXUHO\ RQH RI WKH RXWVWDQGL KDYLQJ PRYHG EHWZHHQ ZRUN LQ WKH LQIRUPDWLRQ L SURIHVVRUVKLSV LQ WZR GHSDUWPHQWV RI LQIRUPDWLRQ KLV FDUHHU 3URIHVVRU 2SSHQKHLP KDV SXEOLVKHG ZLG LVVXHV LQ WKH OLEUDU\ DQG LQIRUPDWLRQ SURIHVVLRQ IUHHGRP RI LQIRUPDWLRQ DV ZHOO DV UHVHDUFK HYDOXD RSHQ DFFHVV VFKRODUO\ FRPPXQLFDWLRQ DQG WKH GLJ 'DYLG %DOO +RQRUDU\ 6HFUHWDU\ RI 8.HL* 3LFWXUHV RI

SUHVHQWDWLRQ DQG IXUWKHU GHWDLOV RI ERWK WKH D
ZLQQHUV FDQ EH IRXQG DW [illegible] DZDUGV WRQ\ NHQ

8.HL* LV D 6SHFLDO ,QWHUHVW *URXS RI &,/,3 WKH &KI
,QIRUPDWLRQ 3URIHVVLRQDOV DQG LV D ORQJ HVWDEOLVK
XVHUV DQG GHYHORSHUV RI HOHFWURQLF LQIRUPDWLRQ U
WKH HIIHFWLYH H[SORLWDWLRQ DQG PDQDJHPHQW RI HOHF
BBBB

Chemical Information / Cheminformatics Books

&KHPLFDO ,QIRUPDWLRQ IRU (GXFDWLRQ -RKQ :LOH\ -U &XUUDQR 'DQD / 5RWK 5R\DO 6RFLHW\ RI &K

:H KRSH WR LQFOXGH D UHYLHZ RI WKLV LQ RX

KWWS ZZZ UVF RUJ VKRS ERRNV
KWWS SXEV UVF RUJ HQ FRQWHQW HERRN

,QWURGXFLQJ &KHPLQIRUPDWLFV E\ 'DYLG :LOOLDPV 7KLV ERRN LV DYDLODEOH LQ .LQGOH IRUPDW DV ZHOO DV YHUVLRQ

KWWS OHDUQFKHPLQIRUPDWLFV FRP

BBBB

7KH ILUVW DUWLFOH FRYHUHG DHURJHOV 7KH VSHFLILF D
HQYLURQPHQWDO FOHDQXS DV FORWKLQJ LQVXODWLRQ DQ

& (1 LV DQ LPSRUWDQW $&6 PHPEHU EHQHILW WKDW LV DY
PHPEHUV ZRUOGZLGH WKURXJK LWV SULQW DQG HOHFWUF
FHQ DFV RUJ

&$6 7UDLQLQJ LQ WKH 8.
,Q DGGLWLRQ WR WKH H OHDUQLQJ UHVRXUFH &$6 /HDU
WUDLQLQJ VHVVLRQV IRU ERWK 671Š DQG 6FL)LQGHUŠ LQ W

:H DUH DOVR DEOH WR FRQGXFW µLQ KRXVH¶ WUDLQLQJ VH
RI &$6 EDVHG 671 RU 6FL)LQGHU VHDUFKLQJ $OVR LI \RX
WKH &$6 SURGXFWV RU ZRXOG OLNH IXUWKHU LQIRUPDWL
SOHDVH FRQWDFW XV DW FDV#FDV RUJ
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STN News

&RQWULEXWHG E\ 'U $QQH -RQHV &$6 $SSOLFDWLRQV 6SHF

$QQXDO 0(Š/,1(Š 1HORDG RQ 671 1HZ 6HDUFKLQJ &DSDE
8SGDWHG 0H6+ 7KHVDXUXV
7KH DQQXDO UHORDG RI 0('/,1(RQ 671 ODXQFKHG RQ -D
LQFOXGHV WKH 0H6+ 0HGLFDO 6XEMHFW +HDGLQJV
LQFOXGH

- 0XOWLSOH DXWKRU DIILOLDWLRQV ± 2UJDQL]DWLRQDO
  QRZ SURYLGHG IRU DOO DXWKRUV UDWKHU WKDQ MXVW
  - %,% DQG $// GLVSOD\V KDYH EHHQ XSGDWHG WR LQ
    LQIRUPDWLRQ
  - 7KH QHZ $8 &6 FXVWRP GLVSOD\ IRUPDW SURYLGH
    VRXUFH LQIRUPDWLRQ SHU UHFRUG
- 8QLTXH DXWKRU LGHQWLILHUV IURP WKH 25&,' 5HJLVW
- ([SDQGHG FLWLQJ GRFXPHQW VHDUFK DQG GLVSOD\
  K\SHUOLQN WR FLWLQJ GRFXPHQWV RI LQWHUHVW
- 1HZ *UDQW 2UJDQL]DWLRQ *2 DQG *UDQW 1XPEHU *1
  WKH LQVWLWXWLRQV IXQGLQJ PHGLFDO DQG VFLHQWLI
- 7KH QHZ $EVWUDFW /DQJXDJH $%/$ ILHOG SURYLGH
  ZKLFK WKH SXEOLVKHU SURYLGHG DQ DEVWUDFW

)RU IXUWKHU LQIRUPDWLRQ RQ WKH HQKDQFHPHQWV HQWH
BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB

SciFinder News

&RQWULEXWHG E\ 'U $QQH -RQHV &$6 $SSOLFDWLRQV 6SHF

&$6 DQG 3HUNLQ(OPHU $QQRXQFH &ROODERUDWLRQ
7KH DQWLFLSDWHG H[FOXVLYH &KHP%LR'UDZ LQWHUIDFH
FROODERUDWLYH HIIRUW EHWZHHQ &$6 DQG 3HUNLQ(OPHU

7KLV IHDWXUH DOORZV &KHP%LR'UDZ 8VHUV YHUVLRQ XV
ZLWKLQ WKH &KHP%LR'UDZ LQWHUIDFH DQG WKHQ EH WD
UHVXOWV ZLWKLQ 6FL)LQGHU 7KLV GHYHORSPHQW ZLOO E
HQKDQFHPHQW IRU XVHUV RI ERWK 6FL)LQGHU DQG &KHP%L

56& &,&$* 1HZVOHWWHU 6XPPHU

&RQWULEXWHG E\ 6WHSKDQLH 1RUWK $OO\O &RQVXOWLQJ

6SULQJHU %RRN $UFKLYHV 5HOHYDQW 6FLHQWLILF 5HVHDU

7KH 6SULQJHU %RRN $UFKLYHV LV D SURMHF
6SULQJHU ERRNV SXEOLVKHG VLQFH WKH V
DFFHVV WR SDVW VFLHQWLILF OLWHUDWXUH
IRU 5 ':LWK DQ DGGLWLRQDO H%RRNV UH
WKH 6SULQJHU %RRN $UFKLYHV WKH FROOHF
WKDQ (QJOLVK WLWOHV DQG *HUPDQ ODQJXDJH V
LQFOXGH PRUH WKDQ &KHPLVWU\ UHODWHG KLVWRUL

,)/$:RUOG /LEUDU\ DQG ,QIRUPDWLRQ &RQJUHVV $FTX
'HYHORSPHQW 6HFWLRQ 2SHQ $FFHVV FRQYHUJLQJ RQ &RC
WK QG $XJXVW /\RQ)UDQFH
KWWS FRQIHUHQFH LIOD RUJ LIOD FDOOV IRU SDSHUV RS
GHYHORSPHQW

,QWHUQDWLRQDO 'DWD DQG ,QIRUPDWLRQ 0DQDJHPHQW &R
WK6HSWHPEHU RXJKERURXJK
KWWS LGLPF RUJ

WK &RQIHUHQFH RQ 2SHQ $FFHVV 6FKRODUO\ 3XEOLVKLQJ
WK WK 6HSWHPEHU 81(6&2 3DULV
KWWS RDVSD RUJ

2SHQ $FFHVV +RZ LW ZLOO FKDQJH>\8RXHU* SHRXLHVW@RQDO
UG 6HSWHPEHU /RQGRQ
KWWS ZZZ XNHLJ RUJ XN WUDKLQQLQJHY HFKWQRSHQRXFFHVVN

56& ODXQFKHV 0DULQ/LW%HWD DQ RQOLQH YHUVLRQ RI 0D
KWWS EORJV UVF RUJ WHFKQLFDO PDULQOLWEHW

&RPSXWHU PRGHOOLQJ RI PROHFXOHV KDV JDLQHG WKH 1R
WKH WKUHH 1REHOOLVWV 0DUWLQ .DUSOXV RI WKH 8QLYH
8QLYHUVLW\ 86$ 0LFKDHO /HY\ 8QLYHUVLW\ 6FKRRO RI 0HG
DQG $ULHK :DUVKHO RI WKH 8QLYHUVLW\ RI 6RXWKHUQ &D
WKH DZDUG µIRU WKH GHYHORSPHQW RI PXOWL VFDOH PRG
KWWS ZZZ VFLHQWLILF FRPSXWLQJ FRP QHZV QHZVBVWRU

0RQW\ +\DPV IRXQGHU RI 'HUZHQW 3XEOLFDWLRQV DJKDM SD
KWWS G[GRL RUJ M ZSL

7KRPVRQ 5HXWHUV 5HYHDOV 1HZ 6WUDWHJLHV IRU 1DY
3KDUPDFHXWLFDO ,QGXVWU\
:KLWHSDSHU JLYHV LQVLJKW LQWR WHFKQRORJLHV WKDW
'DWD 7KRPVRQ 5HXWHUV 6HS
KWWS WKRPVRQUHXWHUV FRP SUHVV UHOHDVHV 3KD

6SHFLDO ,VVXH &RPPXQLFDWLRQ LQ 6FLHQFH 3UHVVXUHV
6FLHQFH 2FWREHU
KWWS ZZZ VFLHQFHPDJ RUJ VLWH VSHFLDO VFLFRPP LQGH

.HQQHWK 0 0HU] -U QDPHG QHZ (GLWRU

'DVVDXOW 6\VWqPHV DQG $FFHOU\V WR -RLQ)RUFHV
KWWS LQIR DFFHOU\V FRP /(9 .E R7)

'DWD PLQLQJ LQ 8. KLJKHU HGXFDWLRQ LQVWLWXWLRQV O
KWWS ZZZ HOJDURQOLQH FRP YLHZ MRXUQDOV TPMLS

&,1) 6XPPHU &KHPLFDO ,QIRUPDWLRQ 0DWHULDOV LQ
KWWS EXOOHWLQ DFVFLQI RUJ QRGH

[LQGH[$)DQWDVWLF 1HZ ,QGLFDWRU IRU 4XDQWLI\LQJ D
KWWS VFKRODUVKLS EORJVSRW FRP

6FLHQFH &LWDWLRQ ,QGH[6&, FHOHEUDWHV LWV WK DQ
KWWS ZRNLQIR FRP VFL DQQLYHUVDU\ KWPO

+LQGDZL¶V 3URILW 0DUJLQ LV +LJKHU WKDQ (OVHYLHU¶V
KWWS VFKRODUO\RD FRP KLQGDZLV SURILWV DUH

,QYHVWLJDWLQJ MRXUQDOV 7KH GDUN VLGH RI SXEOLVKLQ
KWWS ZZZ QDWXUH FRP GRLILQGHU D

7KH ZLVGRP RI FORXGV
7KH SURPLVH DQG SLWIDOOV RI GRLQJ VFLHQFH ZLWK GLV
&KHPLVWU\ :RUOG 0D\ S
KWWS ZZZ UVF RUJ FKHPLVWU\ZRUOG ZLVGRP FORX

&KHPLVWU\ UHIHUHQFHV LQ WKH GLJLWDO DJH VKDULQJ F
56& 1HZV 0D\ S
KWWS PDJ GLJLWDOSF FR XN IY[UVF UVFQ

'UXJ FRPSDQLHV DUH QRW EHWWHU DW GUXJV
,&,¶V YLVLRQDU\ LQYHVWPHQW ODLG WKH IRXQGDWLRQV
LQGXVWULHV
KWWS ZZZ IW FRP FPV V E G H H IHDEGF

+HDOWKFDUH H[FHOOHQFH JHWV ERRVW IURP IUHH UHVHDU
$ \HDU ORQJ SLORW ZLOO DOORZ VWDII ZRUNLQJ DFURVV
PRVW UHVSHFWHG PHGLFDO DQG VFLHQWLILF MRXUQDOV
KWWS ZZZ MLVF DF XN QHZV KHDOWKFDUH H[FHOOHQFH JL
WULDPD\

1/0 DQG :HOOFRPH /LEUDU\ (VWDEOLVK $JUHHPHQW WR 0D
-RXUQDOV)UHH\ $YDLODEOH 2QOLQH
KWWS ZZZ QOP QLK JRY QHZV ZHOFRPHBOLEUDU\BDJUHHP

('3 2SHQ VXUYH\ UHYHDOV /HDUQHG VRFLHW\ DWWLWXGHV
KWWS ZZZ HGS RSHQ RUJ LQGH[SKS"RSWLRQ FRPBFRQWH