

\$YDLODEOH ~~ZZZQDEKQROD~~WVUHVH DUFKOLEUDU\ FRP

6FKRODUV 5HVHDUFK /LEUDU\

-RXUQDO RI 1DWXUDO 3URGXFW DQG 3ODQW 5HVRXUFHV
KWWS ZZZ VFKRODUVUHVHDUFKOLEUDU\ FRP

,661

,PSDFW RI %DFWHULDO &RQVRUWLD RQ %LRGH
&RQWDPLQDWHG 6RLOV

8PHPD 0RKVLDQGDQ /RZDQX 6KDUPFKLQ .XPDU

'HSDUWPHQW RI =RRORJ\ 0DKDWPD -\RWL 5DR 3KRROH 8QLYH
&HQWUH IRU \$GYDQFHG 6WXGLHV 'HSDUWPHQW RI =RRORJ\ 8

\$%675\$&7

5DSLQGDWUH RI LQGXLVWULDOLJDWLRO XUEDQLJDWLRO DQGHUWRP
KDV EHHQ H[SRQHQLWLD LQFUHDVH LQ QXPEHUV RI DXWRPRELOHV L
VRLO PLFURRUJDQLVPV IRU UHPHGLDWLRO RI SHWUROHXP FRQWDPLQ
ZHUH H[FOXVLYHO\ VHOHFWHG IRU LWV XVH DV D VWDQG IRU KHDY\ V
ZLWKLQ DQG VXUURXQGLQJV RI WKH 7UDQVSRUW 1DJDU -DLSXU 3K\
HIIHFW RI YDULRXV EDFWHULDO FRQVRUWLD ZHUH LQYHVWLJDWHG 5
ZDWHU KROGLQJ FDSDFLW\ LQ WHVW VDP SOHV 7 7 DQG 7 ZHUH
KRZHYHU VKRZHG KXJH HOHYDWLRO 3 LQ DOO WCUHH WHVW V
PJ J PJ J DQG PJ J UHVSHFWLYHO\ :LGH UDQJHV RI
FKDLQ DQG ORQJ FKDLQ DONDQHV ZHUH IRXQG LQ WHVW VDP SOHV
EDFWHULDO FRQVRUWLD ,Q WHVW VDP SOH 7 LQWHUPHGLDWH FRPS
FRQVRUWLXP ' DQG (\$PRQJ WKHVH WKRGH &RQVRUWLD RI FRQVWILQ
H[FHSWLRODO JURZWK IURP UG GD\ RQZDUG \$W WK GD\ RI LQFXE
ZKLFK ZDV QHDO\ IROGV JUHDWHU WKDQ RWKHU FRQVRUWLD 2>
XVDEOH DQG IXQFWLRODO ELRUHPHGLDWLRO WRRO WR LPSURYH VR
GHJUDGDWLRO RI SHWUROHXP K\GURFDUERQ

.H\ZRUGLV FURELDO ELRUHPHGLDWLRO 3HWUROHXP K\GURFDUERQ 6RL

,1752'8&7,21

:LWK H[SRQHQLWLD GHYHORSPHQW RI LQGXLVWU\ DXWRPRELOHV DQ
JUHDWO\ LQFUHDVHG 1HYHUWKHOHV SOHQW\ RI SHWUROHXP ZDV V
GLVSHQVDWLRO DQG LW UHVXOWHG LQ VLJQLILFDQW HQYLURQPHQW
'XH WR FRPSOH[LW\ LQYROYHG LQ WKH WUDQVSRUWDWLRO RI VRLOV
VLWH ELRUHPHGLDWLRO DV WKH VROH PHWKRQ RI WUHDWPHQW %LR
WKH SROOXWDQWV ,W LV DQ HIIHFWLYH ORZ FRVW DQG HQYLURQPH
WKH HQYLURQPHQW > @

\$ONDQHV DUH VDWXUDWHG K\GURFDUERQV ZKHUHDV XQVDWXUDWHG
FDUERQ GRXEOH ERQGV DQG RU WULSOH ERQGV VXFK DV DONHQHV F
HTXDO IRU ERWK VDWXUDWHV DQG XQVDWXUDWHV 5DWHV RI SHWUR
KLJKHVW IRU VDWXUDWHV :KHUHDV KLJK PROHFODU ZHLJKW DURPD
GHJUDGDWLRO > @ \$OWKRJK WKLW SDWWHUQ LV QRW XQLYHUV
QDSKWKDOHQH WKDQ RI KH[DGHFHQ LQ ZDWHU VHGLPHQW PL[WXUH
H[WHQVLYH ELRGHJUDGDWLRO RI DON\O DURPDWLFV LQ PDULQH VHGL

6FKRODUV 5HVHDUFK /LEUDU\

%LRGHJUDGDWLRQ DV ZHOO DV ELRUHPHGLDWLRQ E\ VHOHFWHG E
 UHVWRUDWLRQ RI SROOXWHG HQYLURQPHQWV > @ %LRDYDLODELO
 LQKDELWHG PLFURRUJDQLVPV SOD\ LPSRUWDQW UROHV LQ ELRUHPH
 QDWXUDO FRPPXQLWLHV UHIOHFW LQWHUDFWLRQV EHWZHHQ PLFURE
 VKDULQJ RI QXWULWLRQDO UHVRXUFHV LV FRPPRQ > @ DQG LQWH
 JURZWK DQG ELRGHJUDGDWLRQ > @ ,W KDV DOUHDG\ EHHQ VKRZQ
 W\SHV RYHUFRPHV LQFRPSDWLELOLWLHV LQ GHJUDGDWLRQ RI GLYHU
 ,Q WKLV VWXG\ ZH XVHG IRXU QDWLYH VRLO PLFURRUJDQLVPV IRU
 ,QGLD 7HVW VLWHV H[DPLQH LQ WKLV VWXG\ ZHUH H[FOXVLYHO\ V
 KHDY\ WUDQVSRUW YHKLFOHV

0\$7(5,\$/6 \$1' 0(7+2'6

6DPSOH FROOHFWLRQ

6XUIDFH VRLO FP GHWSK ZDV FROOHFWHG IURP WKH DUHDV ZLW
 1 (1 (DQG 1 (IURP
 JDUDJHV IXHO VWRUDJH WDQNV DQG DW KHDY\ YHKLFOH VWDWLRQ
 GXULQJ WKH GD\ WR GD\ DFWLYLW\ DQG XVHV RI IXHOV PDLQO\ RI Z
 IURP VLWH FRPSOHWHO\ LVRODWHG IURP URDGZD\V DQG QRW DFFHVV
 PP VLHYH 7KH SURFHVVHG VDPSOHV ZHUH VWRUH LQ VWHULOH SRO

Table 1: 6DPSOHV FROOHFWHG IRUP IROORZLQJ VLWHV DQG WKHLU

6DPSOH 6LWHV	\$EEUHYLDWLRQ &RQWURO
6XUDMSRO %D]DU 5G \$QDM 0DQGL	T1
.ULVKQD 0DUNHWLQJ /DO 'XQJUL	T2
9LMD\ 3DWK /DO 'XQJUL	T3

3KIVLRFKHPLFDO FKDUDFWHUL]DWLRQ RI VRLO

'HWHUPLQDWLRQ RI ZDWHU KROGLQJ FDSDFLW\
 :+& ZDV GHWHUPLQH DFFRUGLQJ WR .QHHU 5DFN]RZVNL ER[EULHIO
 ILOOHG ZLWK VRLO 7KH VRLO ILOOHG ER[LV WKHQ NHSW LQ D ELJ
 EHQHDK ([FHVV ZDWHU LV WKHQ DOORZHG WR GUDLQ RXW DQG WKH
 (VWLPDWLRQ RI FDUERQDWH DQG ELFDUERQDWH LQ VRLO
 &DUERQDWH DQG ELFDUERQDWH ZDV HVWLPDWHG E\ VLPSOH DFLG
 S+! DQG ODWHU LQ WKH SUHVHQFH RI PHWK\O RUDQQH S+ LQ
 (VWLPDWLRQ RI FKORULGH LQ VRLO
 &KORULGH GHWHUPLQDWLRQ LV EDVHG RQ WKH IRUPDWLRQ RI QHDU
 ZLWK VLOYHU QLWUDWH > @
 (VWLPDWLRQ RI FDOFLXP FDUERQDWH
 7KH DPRXQW RI +&O XVHG LQ UHDFWLQJ ZLWK FDOFLXP FDUERQDWH
 SKHQROSKWKDOHLQ DV DQ LQGLFDWRU > @
 (VWLPDWLRQ RI RUJDQLF PDWWHU DQG RUJDQLF FDUERQ LQ VRLO
 2UJDQLF PDWWHU DQG RUJDQLF FDUERQ LQ VRLO ZDV GHWHUPLQ
 %ULHIO\ D ZHLJKW RI J RI VRLO ZDV WDNHQ &QWRQDQ P@FR

6WDWL VWLFDO HYDOXDWLRQ

7KH PHDQ YDOXH ZHUH FRPSDUHG XVLQJ UHVSHFWLYH VWDQGDUG FRQWURO DQG WHVW VDP SOHV IRU HYDOXDWLRQ RI VLJQLILFDQFH WHVW RU \$129\$ WHVW 3 ZDV FRQVLGHUHG DV VLJQLILFDQW 5(68/76

3KIVLRFKHPLFDO FKDUDFWHULJDWLRQ

6DPSOHV ZHUH FROOHFWHG IURP WKUHH VHSODUDWH VLWHV DURXQG YDULRXV SDUDPHWHUV YL] S+ HOHFWULFDO FRQGXFWLYLW\ DYDLO PDWWHU VRLO RUJDQLF FDUERQ WRWDO GLVVROYHG VROLGV FKOR 7DEOH VKRZV FRPSDUDWLYH PHDVXUHPHQW RI DERYH SDUDPHWHUV

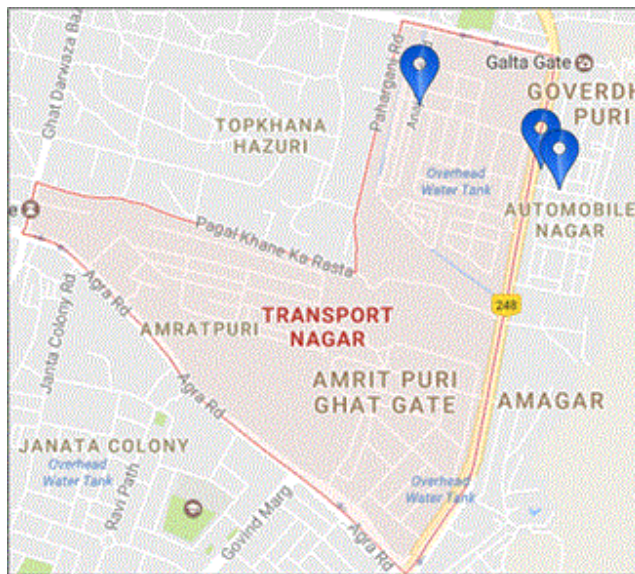


Figure 1: 6LWH IURP ZKHUH VDP SOHV ZHUH FROOHFWHG

5HVXOW VKRZ WKDW S+ HOHFWULFDO FRQGXFWLYLW\ ELFDUERQDWH ZHUH VXEVWDQWLDQ\ UHGXFHG ,Q 7 WKH ZDWHU KROGLQJ FDSDFL ZDV REVHUYHG LQ 7 DQG 7 /HYHO RI S+ LQFUHDVHG WR DOPRVW RI RI FRQWURO ,Q FRQWURO VDP SOH ELFDUERQDWH ZDV HVWLPDV 3 WKDQ 7 7 DQG 7 HVWLPDWHG DV PJ J PJ J DC 6RLO RUJDQLF PDWWHU VRLO RUJDQLF FDUERQ WRWDO GLVVROYHG VDP SOHV 7 7 DQG 7 FRPSDULQJ WR FRQWURO 0HDVXUHPHQW RI LQ DOO WKUHH WHVW VDP SOHV 7 7 DQG 7 ZKLFK ZDV FDOFXODW UHVSHFWLYHO\ ,Q FRQWURO VDP SOH FKORULGH ZDV HVWLPDWHG DV ZDV REVHUYHG LQ 7 7 DQG 7 & 1 UDWLRV LQ WHVW VDP SOHV 7 FRQWURO 7DEOH

Table 3: 3KIVLRFKHPLFDO FKDUDFWHULJDWLRQ RI FRQWURO DQ

3DUDPHWHUV	8QLW	&RQWURO	7	7	7
S+	-	6.36	7.95	7.85	7.82
(OHFWULFDO &RQGXFWLYLW\	ms ⁻¹	2.8	1.48	1.6	2.24
\$YDLODEOH &DUERQDWH	mg/100 g	-	-	-	-
%LFDUERQDWH	mg/100 g	610	152.5	122	122

&DOFLXP &DUERQDWH mg/100 g	1	1.5	1	0.5
6RLO 2UJDQLF 0DWWHU %	0.103	0.413	0.31	0.413
6RLO 2UJDQLF &DUERQ %	0.06	0.24	0.18	0.24
7RWDO 'LVVROYHG 6ROLGppt	0.251	0.888	0.954	1.33
&KORULGH mg/100 g	4.2	53.9	71	146.26
:DWHU +ROGLQJ &DSDFLW%	24.66	18.98	14.24	16.98
ORLVWXUH &RQWHQW %	0.13	0.431	0.502	0.644
& 1 5DWLRQ	4:01	21:01	17:01	16:01

7RWDO SHWUROHXP KIGURFDUERQ

*DV FKURPDWRJUDSK\ PDVV VSHFWURPHWHU DQDO\VVH RI WKH UHVL DQG 7 FRPSDUHG ZLWK FRQWURO VDPSON)LJXUH 7KH REWDLQH RI FRPSRXQGV LW ZDV UHYHDOHG WKDW 73+ LV LQFUHDVHG VXEVWL VDPSON

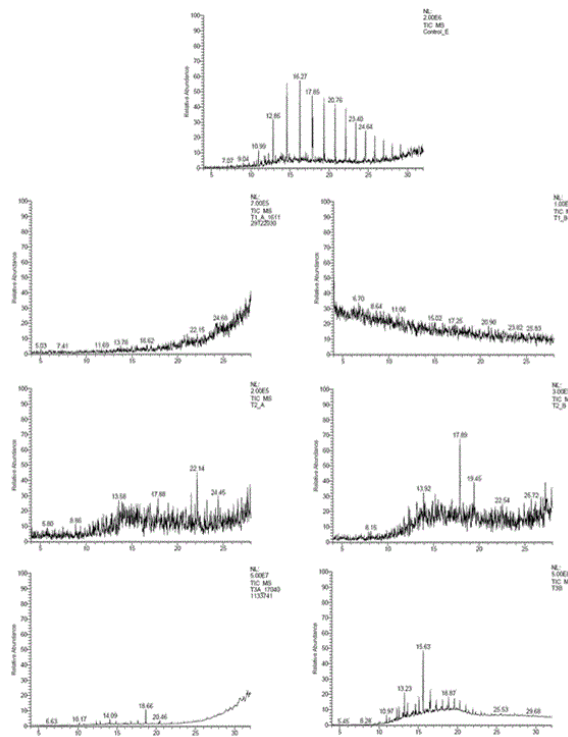


Figure 2: * & 06 FKURPDWRJUDPV RI FRQWURO D 7 \$ 7 % E F 7 \$ 7 % G FROOHFWHG RQ ILUVW GD\ % 6DPSOH IROORZLQJ WUHDWPHQ

:LGH UDQJHV RI DONDQHV & WR & LQFOXGLQJ ERWK VKRUW FKDI XQGHFDQH & EURPR GRGHFDQ & 7ULPHWK\OGRGHFDQH PHWK\O QRQDGHFDQH & GLGHF\O HLFVRDQH & KHQHLFRVDQH RFWDFRVDQH & DQG Q QRQDFRVDQH & WKDW ZHUH SUHVHQW L K\GURFDUERQV DQG 3\$+V ZHUH GHWHFWHG)URP WKH YDULRXV G FRQVRUWLXP ZDV DEOH WR SDUWLDOO\ GHJUDGH VRPH RI WKHP 7DE

Table 4: Compounds identified in control sample with its respective retention time

57	& R P S R X Q G V
	1,5-Diphenyl-hex-3-ene
	Decane, 3-bromo
	Benzenepropanol, propanoate
	1-Methylamino-2-[(1-methyl-2-benzimidazolyl)methylamino]benzene
	1,4,8-Metheno1Hcyclopent[f]azulene
	Pentanoic acid, 1,1-dimethylpropyl ester
	Methyl-2-(methoxycarbonyl)-3-methyl-5-phenylpent-4-enoate
	Ethaneperoxoic acid, 1-cyano-2-methyl-1-phenylpropyl ester
	1-Deoxydarabinitol tetrakis (trifluoroacetate)
	Undecane, 4,7-dimethyl
	2-Azetidinone, 3,3-dimethyl-4-phenyl-1(phenylethyl)
	2,3,4-Trifluorobenzoic acid, 2-fluorophenyl ester
	4-Hydroxy-5,6-epoxyáionone
	10-Methylnonadecane
	2,3,4-Trifluorobenzoic acid, 2-naphthyl ester
	4-Butyl-6-ethyl-5-methyl-2-Hpyran-2-one
	10-Methylnonadecane
	2,2,5-Trimethylhexan-4-one
	Heptanamide, N-(2-cyanoethyl) N-hexyl
	6-Tetradecanesulfonic acid, butyl ester
	5-Iodononane
	Diphosphorous tetrafluoride
	Methyl N-trifluoroacetyl-S-(prolyl-2-pyrrolidineacetate)
	3,3-dimethylbutyric acid, 2,2,2-trifluoroethyl
	Oxalic acid, 6-ethyloct-3-yl isobutyl ester
	Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpentyl)
	Decane, 3-bromo
	Pyridine, 3[(1,1-dimethylethyl)thio]
	6-Tetradecanesulfonic acid, butyl ester
	Sulfurous acid, decyl-2-propyl ester
	Phosphonic acid, bicyclo[2.2.1]hept5en2yl, dimethyl ester
	Decane, 3-bromo
	Borane, diethyl(decyloxy)
	1,1-Dimethylpropyl-2-ethylhexanoate
	Sulfurous acid, butyl isohexyl ester
	1(5'methylfurfuryl) pyrrolidine
	Decane, 3-bromo
	3-Buten-2-one, 4-(1,2-dihydroxy-2,6,6-trimethylcyclohexyl) [1à,1(E),2á]
	Cis-1-methyl-3-nonylcyclohexane

	3,4-Hexanedione, 2,2,5-trimethyl
	Butyltertbutylisopropoxyborane
	Sulfurous acid, cyclohexylmethyl nonyl ester
	Butane, 2-azido-2,3,3-trimethyl
	O-Butyl, O-1,2,2-trimethylpropyl methylphosphonate
	2,6-Dodecadienoic acid, 10(bromoacetoxy)-11-methoxy-3,7,11-trimethyl, methyl ester
	t-Butyl cyclopentaneperoxy-carboxylate
	DL-4,5-Octanediol
	2-Amino-octadecane-1,3,4-triol-1,3:2,4-bismethaneboronate
	Meso-2,5-Dimethyl-3,4-hexanediol
	9-Phenanthrenemethyl-2,6-dimethylbenzoate

Table 5: & R P S R X Q G V L G H Q W L I L H G L Q 7 Z L W K L W V U H V S H F W L Y H U

57	& R P S R X Q G V
	Cyclohexane-1-carboxamide, 4-methyl-N-(4-tolyl)
	3-Cyclohexene-1-ethanol, ðæthenylà, 3-dimethyl-6-(1-methylethylidene)
	Trans-3-methylpent-3-ene-5-ol
	Cyclohexanol, 2-bromo, trans
	3,6-Epoxy-2H, 8H-pyrimido[6,1b][1,3]oxazocine-8,10-(9H)dione,3,4,5,6-tetrahydro-11-methyl-14[[trimethylsilyloxy],[3R(à,4á,6á)]]
	N(7,7-Dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)ethanesulfonamide
	Succinic acid, di(2-ethylcyclohexyl) ester
	Bis(2-ethylbutyl) diselenide 23.95 3,4Hexanedione, 2,2,5-trimethyl
	Azetidine, 1-benzyl-2,2,3,3-tetramethyl
	2,2-Dimethylpropyl-2,2-dimethylpropanesulfonyl-sulfone
	1,4-Bis(methylsulfonyl)piperazine
	1,3-Benzenediol, O-cyclobutanecarbonyl-O'(3-fluorobenzoyl)
	1H-Pyrrole-2-carboxamide, 4-amino-N-(3-amino-3-iminopropyl) 1-methyl
	Propane, 1,1,2,2-tetrakis(difluorophosphino)
	1-Amino-1, 3-bis-(4-amino-6-dimethylamino-2-yl)propane
	3-Hexene, 1,1'[ethylidenebis(oxy)]bis, (Z,Z)
	2,2-Dimethylpropyl 2,2-dimethylpropanethiosulfinate
	4-Nonene, 2,3,3-trimethyl, (Z)
	Cyclopropane, 1-bromo-1-chloro-2-fluoro
	Ether, hexyl pentyl
	10-Hydroxy-2,2,9,9-atetramethyl-1,2,5a, 6,7,8,9,9a-octahydro-1,4-methano-3-benzoxepin-5(4H)one
	Acetic acid, trifluoro, lithium salt
	1-Hexyl-2-nitrocyclohexane
	2(1-Methylcyclopentyl)oxy tetrahydropyran

1-Cyclohexyl-1-(4-ethylcyclohexyl) ethane
N(7,7-Dimethyl-2-oxobicyclo[2.2.1]hept-1-yl) methanesulfonamide
2(Cyclohexylimino)-3,3-dimethylbutane
Decane, 3-bromo
1-Hexyl-2-nitrocyclohexane
2-Pentene, 5-bromo-2,3-dimethyl
1-Hexyl-1-nitrocyclohexane
Bicyclo[3.2.0]heptan-3-one, 2-hydroxy-1,4,4-trimethyl, O-acetyloxime
Butanamide,2-(dimethylamino)N[7[(4-hydroxyphenyl)methyl]3(1-methylethyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]3-methyl
1-Cyclohexylnonene
Sulfurous acid, octadecyl-2-propylester
Cyclopropane, 1-(1-methylethyl)-2-nonyl
Butanoic acid, 2-methyl, 3-methylbutyl ester
trans-4-tertbutylcycloheptanol
Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpentyl)
Cyclohexane, 1,1'[1,2-bis(1,1-dimethylethyl)1,2-ethanediyl]bis,(R*,R*)(ñ)
1-Hexyl-2-nitrocyclohexane
Cyclohexanol, 4-ethyl-4-methyl-3-(1-methylethenyl),(1à,3à,4à)
O-Methyl,bis(O-1,2,2-trimethylpropyl)phosphate
Cyclohexane, 1,1'[1,2-bis(1,1-dimethylethyl)1,2-ethanediyl]bis,(R*,R*)(ñ)
Pyrrolidine, 1-(1-oxo-1,4-methyl-8-hexadecenyl)
1-Hexyl-2-nitrocyclohexane
Cis-1-methyl-3-n-nonylcyclohexane
3-Methyl-1[(1H)-1,2,4-triazol-1-yl]butan-2-one
Pentyl glycolate

Table 6: & R P S R X Q G V L G H Q W L I L H G L Q 7 Z L W K L W V U H V S H F W L Y H U

57	& R P S R X Q G V
	5-(Indole-3-yl)methyl-2-thioxoimidazolidin-4-one
	1,1,4,4,7,7,10,10,13,13,16,16-Dodecamethyl-1,4,7,10,13,16-hexasilacyclooctadeca-2,5,11,14-tetrayne
	Bicyclo[2.2.2]oct-2-ene, 1,4,5,5,6,6-hexafluoro
	Benzene, [2(methylsulfonyl)1-propenyl]
	2,2-Dimethylpropyl-2-dimethylpropanesulfinyl sulfone
	2-Butanone, 3-chloro-4-hydroxy-1,4-diphenyl
	4,5-Dichloro-N[(1,2,3,4-tetrahydroisoquinolin-2-yl) methyl]phthalimide
	Ethanediamide, N,N'bis(1phenylethyl)
	Octanamide, N(4-chlorophenyl)
	Bis(trifluoromethylsulfonyl)methane

N,N-Dibutyl-3-coumarine carboxamide
1-Butene,1,1,2,3,3,4,4,4-octafluoro
2,4-Imidazolidinedione, 1,3,5-trimethyl-5-phenyl, (ñ)
1-Phenyl-2-methyloct-1-ene
Oxetane, 2,2,3,3-tetramethyl-4,4-diphenyl
Urea, N,N'di2-propenyl
Benzenehexanenitrile, á,ádimethylíoxo
Cis-2-Nitro-4-butylcyclohexanone
Diborane(4)tetramine, octamethyl
Benzeneacetamide, ãethyl-N-formyláhydroxy
5-Hepten-3-one,5-ethyl-2-methyl
4-Butyl-5-methylpyrazalone
Butanoic acid, 2-methyl, 2-methylbutyl ester
2-Heptanone, 7-bromo1phenyl
1H-Imidazole,1(1-oxopentyl)
Methapyrilene metabolite
n-Butyl cyanoacetate
3-Oxobutan-2-yl 2-methylbutanoate
Propane, 2[(1,1-dimethylethyl)sulfonyl]2-methyl
2-Morpholino-4H-5,6-benzothiazin-4-one
7-Acetyl-2-hydroxy-2-methyl-5-isopropylbicyclo[4.3.0]nonane
1,3-Benzenediol,O,O'di(cyclohexanecarbonyl)
9-Phenanthrylmethyl-3-methoxybenzoate
Fumaric acid, 2-pentyl propyl ester
2-Thiophenecarboxylic acid, 4-isopropylphenyl ester
4H-Pyrido[1,2a] pyrimidine-3-acetic acid, 8-methyl-4-oxo, ethyl ester
2,5,5-Trimethyl-2-oxo1,2,3-dioxophosphorinane
Fumaric acid, di(3,5-dimethylcyclohexyl) ester
Carbonic acid, ethyl 3-(1-methylethoxy) phenyl ester
1,5-Bis(trifluoromethyl)pentasulfide
4,5-Dihydro-N-phenyl-3-furamide
Menadiene monopmethoxybenzoylhydrazone
Furan-2-carboxylic acid (cyanodimethylmethyl) amide
Cycloheptene, 5-bromo
(E)2-Hydroxyimino-3-oxobutyric acid, 1,1-dimethylethyl ester
(5aá,9aá,9bá)5,5a,6,7,8,9,9a,9b-octahydro-6,6,9a-trimethyl naphtho[1,2c]furan1(3H)one(drimenin)
Benzamide, N(4-cyanomethylphenyl) 4-fluoro
transCinnamyl tiglata
1,3-Bis(cyclopentyl)-1-cyclopentanone
2-(4-Bromobutyl) furan

Table 7: & RPSRXQGV LGHQWLILHG LQ 7 ZLWK LWV UHVSHFWLY

57	& RPSRXQGV
	Sulfurous acid, 2-ethylhexyl tridecyl ester
	Sulfurous acid, 2-ethylhexyl hexyl ester
	Hexadecane, 2,6,10,14-tetramethyl
	1-Methyl-4-isopropylcyclohexyl 2-hydroperfluorobutanoate
	Sulfurous acid, butyl nonyl ester
	Muurolane B
	1-Hexyl-2-nitrocyclohexane
	1,4-Methanonaphthalene-2,2,3,3-tetracarbonitrile, 1,4-dihydro-9-(1-methylethylidene)
	4-Propionyloxypiperidine
	Oxalic acid, isoheptyl neopentyl ester
	Decane, 3-bromo
	10-Methylnonadecane
	Pentanoic acid, 1,1-dimethylpropyl ester
	6-Tetradecanesulfonic acid, butyl ester
	Sulfurous acid, butyl nonyl ester
	Pentadecane, 2,6,10-trimethyl
	Sulfurous acid, butyl nonyl ester
	Pentadecane, 2,6,10,14-tetramethyl
	Decane, 3-ethyl-3-methyl
	Sulfurous acid, butyl nonyl ester
	Borane, diethyl(decyloxy)
	Eicosane
	Sulfurous acid, butyl nonyl ester
	Oxalic acid, isoheptyl neopentyl ester
	17,21-Dimethylheptatriacontane
	Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpentyl)
	Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpentyl)
	17,21-Dimethylheptatriacontane
	Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpentyl)
	6-Tetradecanesulfonic acid, butyl ester
	17,21-Dimethylheptatriacontane
	17,21-Dimethylheptatriacontane
	Cyclohexane, 1(1,5-dimethylhexyl)-4-(4-methylpentyl)
	17,21-Dimethylheptatriacontane
	Cyclohexane, 1(1,5-dimethylhexyl)-4-(4-methylpentyl)

6-Tetradecanesulfonic acid, butyl ester
17,21-Dimethylheptatriacontane
17,21-Dimethylheptatriacontane
17,21-Dimethylheptatriacontane
Cyclohexane, 1(1,5-dimethylhexyl)-4-(4-methylpentyl)
17,21-Dimethylheptatriacontane
Meso-3,4-Dicyclohexyl-2,2,5,5-tetramethylhexane
Meso-3,4-Dicyclohexyl-2,2,5,5-tetramethylhexane
17,21-Dimethylheptatriacontane
6-Tetradecanesulfonic acid, butyl ester
17,21-Dimethylheptatriacontane
17,21-Dimethylheptatriacontane
6-Tetradecanesulfonic acid, butyl ester
9-Hexacosene
17,21-Dimethylheptatriacontane

Effect RI EDFWHULDO FRQVRUWLD RQ VRLO

\$IWHU GD\ V WUHDWPHQW ZLWK YDULRXV FRQVRUWLXP QHZ SHDNV 7KXVH SHDNV ZHUH IXUWKHU FRPSDUHG ZLWK FRQWURO WR HQVXUH LQWHUPHGLDWH FRPSRXQGV ZHUH REVHUYHG VXFK DV +\GUR EURPRDFHWR\ PHWKR\ WULPHWK\O PHWK\O HVWHU DQG /LNHZLVH LQ 7 RQH LQWHUPHGLDWH FRPSRXQG ZDV IRXQG L H QHZ SHDNV ZHUH REVHUYHG LQ FKURPDWRJUDP WKXVH ZHUH IXUWKH 8QGHFDQH GLPHWK\O 7HWUDGHFDQHVXOIRQLF DFLG EXW\O HVV

Table 8: &RPSRXQGV DQG LQWHUPHGLDWH FRPSRXQGV IRXQG LQ WHVW VDPSONH RQ ILUVW GD\ % 6DPSOH IROORZLQJ WUHDWPHQW ZLWK ED

&RQWURO WR 7		&RQWURO WR 7		&RQWURO WR 7	
7 \$	7 %	7 \$	7 %	7 \$	7 %
Decane, 3-bromo	Decane, 3-bromo	-	Decane, 3bromo	Decane, 3-bromo	Decane, 3-bromo
3,4-Hexanedione, 2,2,5-trimethyl	4-Hydroxy-5,6-epoxyáionone	-	2,2,5-Trimethylhexan	Pentanoic acid, 1,1-dimethylpropyl ester	Pentanoic acid, 1,1-dimethylpropyl ester
Cyclohexane, 1(1,5-dimethylhexyl)-4-(4-methylpentyl)	2,6-Dodecadienoicacid, 10-(bromoacetoxy)11-methoxy-3,7,11-trimethyl, methyl ester	-	-	10-Methylnonadecane	Undecane, 4,7-dimethyl
-	t-Butylcyclopentaneperoxycarboxylate	-	-	10-Methylnonadecane	6-Tetradecanesulfonic acid, butyl ester
-	-	-	-	Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylpentyl)	Borane, diethyl(decyloxy)

'HJUDGDWLRQ RI SHWUROHXP KIGURFDUERQ EI EDFWHULDO FRQVRUWLD

\$ WRWDO RI ILYH GLIIHUHQW FRQVRUWLD ZHUH XVHG WR HYDOXDWH FRQVRUWLD \$ (FRQVRUWLD \$ FRQWDLQH DDO IRXU LVRODWHV ZK , DQG , UHVSHFWLYHO\

5HVXOW VKRZHG WKDW IROORZLQJ LQRFXDWRQ ZLWK YDULRXV FR
 REVHUYHG 7KH EHVW UHVXOW ZDV UHFRUGHG IRU FRQVUWLXP ' ZK
 WK GD\ RI LQFXEDWLRQ JURZWK RI FRQVUWLXP ' UHDFKHG KLJKHV
 FRQVUWLXP %HVLGHV FRQVUWLXP ' FRQVUWLXP & VKRZHG D FR
 &RQVUWLXP %DQG & UHVSRRGHG HTXDOO\ ZKLFK JUHZ FRQVWDQWO
 IROORZLQJ WK GD\ RI LQFXEDWLRQ &RQVUWLXP \$ ZLWK KLJKHVW
 JURZWK ZDV RQO\ PRPHQWULO\ DQG VKDUSO\ GHFOLQHG IURP WK
 JURZWK LQ FRQVUWLXP \$ ZDV YHU\ FORVH WR WKDW RI FRQVUWLXP

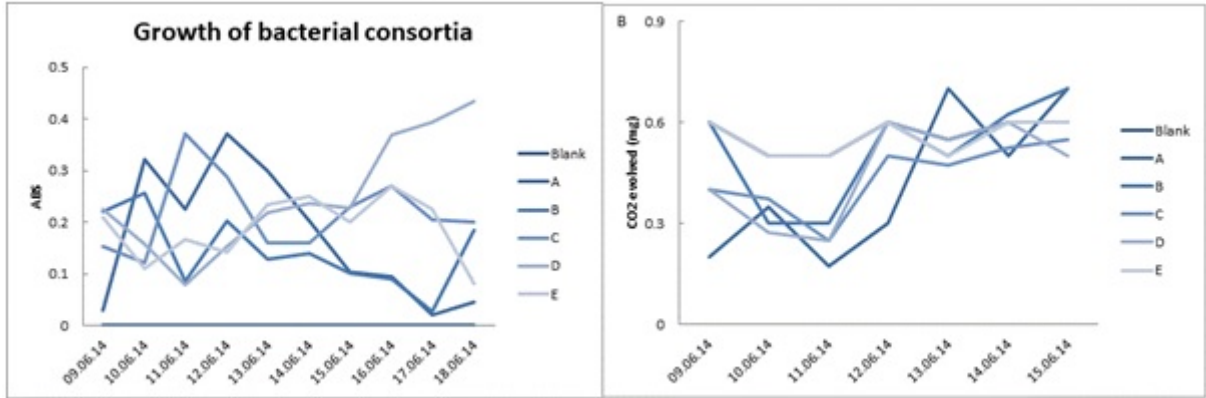


Figure 3: 'HJUDGDWLRQ RI SHWUROHXP K\GURFDUERQ E\ EDFWHULDO FRQVUWLXP
,6&866,21

7KH FXUUHQW UDSLQGDWH RI LQGXVWULDO]DWLRQ DQG XUEDQL]DWLRQ
 WKURXJK KXJH DPRXQW RI ZDVWH WKH\ JHQHUDWH \$XWRPRELOHV FD
 H[SRQHQLDO LQFUHDVH LQ QXPEHUV RI DXWRPRELOHV LQ ,QGLDQV
 DQG JDUDJHV OHDG GHYDWDWLRQ HHHFW RQ SK\VLR FKHPLVWU\ RI
 7KH SUHVHQW VWXG\ VKRZV WKDW WKH SK\VLR FKHPLVWU\ RI VLWHV
 DOO WHVW VLWHV RQH DW 9LMD\ 3DWK /DO 'XQJUL ZDV QRWHG DV
 FKORULGH FRQWHQW VRLO RUJDQLF PDWWHU DQG VRLO RUJDQLF FD
 6LPLODUO\ HOHFWULFDO FRQGXFWLYLW\ ZDV KLJKHU DW WKLV VLWH
 SHUKDSV FDXVHG DEVHQFH RI FURSV DQG RU SODQWV IURP DOO WK
 VDOLQLW\ RI WKH VRLO LV RQH RI WKH PDLQ IDFWRUV WKDW OLPLWV
 7KLV VWXG\ UHSRUWHG KLJKHU S+ LQ DOO WHVW VLWHV ZKLFK ZDV F
 K\GURFDUERQ (DUOLHU VWXGLHV UHSRUWHG VLPLODU FRQWHVW VXF
 VRLO H[HUWV PRUH HHHFW RQ WKH ELRORJLFDO SURFHVV LQ WKH VL
 PLFURELDO PHGLDWHG SURFHVVHV KDYH EHHQ LQYHVWLJDWHG LQ V
 K\GURFDUERQV FDQ EH FDUULHG RXW VXFFHVVIXOO\ DW VDOW FRQ
 LPSURYH WKH DFFHVVLELOLW\ RI VRLO RUJDQLF PDWWHU WR WKH VR
 &KHPLFDQV WKDW RFFXU LQ 73+ JHQHUDOO\ LQFOXGH KH[DQH EHQ]H
 VXP RI 93+ DQG (3+ K\GURFDUERQV UDQJH EHWZHHQ & & DQG & &
 WKLV VWXG\ FRQILUP SUHVHQFH RI PRVW RI WKH (3+V DQG OLPLWH
 SURGXFWV DW WKH VLWHV ,W ZDV REYLRXV IURP WKH UHVXOWV WK
 JUHDWHU DVVHPEODJH RI KHDY\ YHKLFOH DW WKH VLWH ,Q ,QGLD
 FRPSDULQJ WR FRQWURO PRUH SHWUROHXP K\GURFDUERQ ZDV SUHV
 ODUNHWLQJ /DO 'XQJUL 7 QRWHG ZLWK SUHVHQFH RI IXUDQ ZK
 FRXQWULHV)XUDQV DUH FKORULQDWHG SODQDU WULF\FOLF DURP
 LQFOXGHV SRVVLEOH FRQJHQHUV > @ ,QWHUHVWLQJO\ LQ WHVW
 ZLWK PDQ\ SHDNV IRU VLQJOH FRPSRXQG QDPHG DV 'LPHWK\O
 DSSHUHQFH LQ H[D]SHHQDWRQV QRW LQ LQIHUWLOH ZRUNHU
 +DUSHJQDWRQV ,QGLDQ DQW PRVWO\ IRXQG LQ GU\ RSHQ ODQG
 'LPHWK\OKHSDWULDFRQWDOH SHWURODWRQV R\XQGHU DURXQG W

3UHVHGPHU SHJQDOWKDWRDQVR QRWHG LQ RQ HJUDQSWFRMEDFFR@KRWQ
PHDQV SUHDDCGPHW D LV DOVR D SRVVLELOLW\ IRU GHWHFWLRQ RI
VLWH

0LFURRUJDQLVPV SRVVHVV PHFKDQLVPV E\ ZKLFK WKH\ GHJUDGH WK
DQG QLWURJHQ VRXUFHV 7KH SDWWHUQ RI GHJUDGDWLRQ YDULHV
PLFURRUJDQLVPV SRVVHVV GLIIHUHQW FDWDEROL]LQJ HQ\PHV > @
FRQVRUWLD IRU HYDOXDWLRQ RI HILFLHQF\ WR GHJUDGH SHWUROH\
EHVW LQ GHJUDGLQJ SHWUROHXP K\GURFDUERQV DV LW KDV PRVW
3VHXGRPRQGVDLDOREDFQVHDEK SULDJLQGXUJLZHYHU LW ZDV LQWHUHV
FRQVRUWLXP (DOVRXGROKLDQVHGRS SULDJLQGXUJLZHYHU LWK JURZWK ZDV OL
VKRUW VSDQ 7KH RQO\ GLIIHUHQDFKORKEHFWULEREKZDARUW LDRQDSUZV
3KHQ\OREDFRWHUHQVFK ZDV LQ FRQVRUWLXP (DORQJ ZLWK RWKHU
3VHXGRPRQGVDLDOREDFQVHDEK SULDJLQGXUJLZHYHU LWK JURZWK ZDV OL
SHUKDSV QRW3VHFXLRPLGFWDR&S SULDJLQGXUJLZHYHU LWK JURZWK ZDV OL
7KHUH ZDV QR UHIHUHQFH IRXQG WR UHODWH WKLV DVVXPSWLRQ WI
VWXG\

2XU VWXG\ DOVR UHYHDOHG WKDWFRGRPRQGVDLDOREDFQVHDEK SULDJLQGXUJLZHYHU LWK JURZWK ZDV OL
GLG QRW SHUIRUP ZHOO 7KH JURZWK HOHYDWHG LQLWLDOO\ IURP U
FRQVRUWLXP KDG WZR&PKORKEHFWULEREKZDARUW LDRQDSUZV
PHQWLRQHGGKIDQOOREDFWVHQHIEWRUHQHRIH ZDWHU WR JURZ EHVWHU
JURZ ZKLOH LW &DXSRDFHGLH LKWLQ WKDW WKHUH LV SHUKDSV
&DXORKEHFWULEREKZDARUW LDRQDSUZV HYLGHQW E\ JURZWK RI FRQVRU
ZHDNHVW DPRQJ DOO &SULDJLQGXUJLZHYHU LWK JURZWK ZDV OL
EHWZHHQ WKHVH RUJDQLVPV 6LQFH WKLV VWXG\ ZDV H[FOXVLYH QR
WR DVFHUWDLQ WKH VWDWHPHQW

,W ZDV WKHUHIRUH DFFRUGLQJ WR3RKHGPRQGVDLDOREDFQVHDEK SULDJLQGXUJLZHYHU LWK JURZWK ZDV OL
PDQDJLQJ HQGRV\PELRVLV EHWZHHQ LVRODWHV&DXORKEHFWULEREKZDARUW LDRQDSUZV
3KHQ\OREDFRWHUHQVFK VXEVWDQWLDOO\ EHVWHU WKDQ FRQVXRVXPV
VS VXSHULRULW\ RYHU RWKHU PLFURRUJDQLVP LQ GHJUDGLQJ FRPS
IRU GHJUDGDWLRQ DV WKH\ XWLOL]H K\GURFDUERQV LQ WKH SRO\
EDFWHULDO FRPPXQLWLHV KDYLQJ PL[HG SRSXODWLRQ DUH LQYROYH
IRXQG JUDP QHJDWLYH VRLO EDFWHULXP ZLWK WKH DELOLW\ WR GHJ

7KH GHJUDGDELOLW\ RI SHWUROHXP K\GURFDUERQ ZDV HVWLPDWHG
GD\ LQFXEDWLRQ *& 06 ZDV SHUIRUPHG WR VHH LI FRPSOH[K\GURFD
VKRZ WKDW YDULRXV LQWHUPHGLDWHV ZHUH IRUPHG VXFK DV
EURPRDFHWR\ PHWKR\ WULPHWK\O PHWK\O HVWHU DQG
6XUDMSRO %D]DU 5RDG \$QDM 0DQGL 6LPLODUO\ 7ULPHWK\OKH
/DO 'XQJUL /LNHZLVH 8QGDFDQH GLPHWK\O 7HWUDGHFDQ
GLHWK\O GHF\OR\ DW 9LMD\ 3DWK /DO 'XQJUL 7KLV LV WR EH QR
WKHUHIRUH WKH OLWV RI QHZ FRPSRXQG PLJKW FKDQJH LQ ORQJ WH
DQG ORZ PROHFXODU ZHLJKW /0: 3\$+V DFW GLIIHUHQWO\ ZKHQ H[SF
FRPSDUHG WR +0: 3\$+V /0: 3\$+V DUH UHVRQDEO\ PRUH YRODWLOH
PRUH VXVFHSWLEOH WR ELRGHJUDGDWLRQ > @

2XU UHVXOWV VKRZHG WKDW FRQVRUWLXP ' ZDV D FRPSOHWHO\ XVD
SK\VLRFKHPLFDO FKDUFDWHULVWLFV DQG ZLWK HIIHFWLYH ELR GHJ
SURYHV GHJUDGDWLRQ RI FRQWDPLQDQWV LQ WHVW VDPSOHV FROOH

\$&.12:/'(0(17

7KH ZRUN DW RXU ODE LV ILQDQFLDOO\ VXSSRUW E\ WKH 0DXODQD \$]
\$IIDLUV *RYW RI ,QGLD 1HZ 'HOKL ,QGLD

5()(5(1&(6

- > @ (QYLURQPHQW \$JHQF\ 5 ' 3X2E0 LFDWLRQ &/5 /RQGRQ
- > @ %DQNV 0 . 0DOOHGH6R+LODQCG5P 2003WRQRH WDP
- > @ 0LFURELRPH &RPPXQL2W15 (FRORJ\ 6SULQJHU
- > @ *DOOHJR %LRGHHU2000DWL\$Q
- > @)XVH\ 3 DQDU2X\$B0084W %X\$O
- > @ -REVRQ \$ &RRN)' \$QSO:HV 702DENLR\$: 6
- > @ :DONHU - ' &ROZHO&DQ5- DLQ73EIVRUS NLV /
- > @ &RRQH\ - - 6LOYHWL6LURE195R 0 HSN (\$
- > @ -RQHVDU03RO 0983W %X\$O
- > @ :LNVWURP 3 +DJJOXQGLFURE200R0U\$P DQ 0
- > @ 5DR 6 6 DQQQP520NDUS & 6
- > @ %UDJD 5 0 'RXUDGR %UDDPQGLFUREXEMRS : /
- > @ 3HO] 2QYHWRD00199UREISRO
- > @ 9DQ +DPPH -' :DQGL23UREL201%LRWHFKQRO
- > @ 9LJJRU (6YLHWQD06L2002ROOX\$W 5HV
- > @ /DO 5 ,QW ,QVW WUR7\$KL \$JUSL ,EDGDQ 1LJHULD
- > @ 3DQGH\ - 6KDUPD 0 6 2003DVK SXEOLVKLQJ +RXVH
- > @ :DONOH\ \$ DQG %194DFN \$\$ 6RLO 6FL
- > @ 6XEEDLVK % 9 \$QGUSHQW954FLHQ\$H
- > @ 8 6 (3\$ 0HWKRG & 6R[KOHW H[1990FWLRQ 5HYLVLRQ 'HFHP
- > @ 6KDQR+R UOW&7H984KQRS
- > @ 7ULSDW%LR0)HUVV0 6RLOV
- > @ 5LHW] ' 1 DQGR+D\%HLR 009%-LRFKHP
- > @ :DUG ' 0 DQGS%\$URFQYIZUR 078LFURSELRO
- > @ 0XKDPPDG 6 0XOOHU 7 \$DQG (008UURQS/HQ 5 *
- > @ 76'5 3XEOLF +HDOWK 6HUylFH 8 6 'HSDUWPHQW R95+HD06WK D
- > 3%
- > @ &DQDGLDQ &RXQFLO RI 0201V\$HUV RI WKH (QYLURQPHQW
- > @ /LHB1\$000 S
- > @ 1HOVRQ ' 5 6XNNHVWDG /L\$LD028V=D\$OVNLH 5 *
- > @ 3HQHW %LRGHHU2006DWL\$Q
- > @ .\DZ % 0,QGLVD 00 0202URELRS
- > @ =KDQJ %LRHMVBR0117HFKQRS
- > @ %KDWWDFFK\$DUSO (QYHWRD00LFUREISRO
- > @ 3DQQX - . 6LQJK & \$QD-QGLFURELRS