

Supporting Information for

Assessing the combinatorial potential of the RiPP cyanobactin *tru* pathway

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Table of Contents:

Table S1. Successfully expressed mutants described in this study...	2
Table S2. Sequences tested but for which products could not be detected...	5
Table S3A. Analysis of selectivity data and total number of mutations per position...	9
Table S3B. Percent success rate for each amino acid...	10
Table S3C. Percent acceptance of each amino acid at each position, when rules are followed...	11
Table S4. Mass spectral analysis of libraries...	12
S4A. XXIAPFC library...	13
S4B. TSIXPXC library...	26
S4C. TSXXPXC library...	65
S4D. XSXXPXC library...	95

Table S1. Successfully expressed mutants described in this study. *duplicate sequences obtained and correctly expressed twice but not counted twice in statistics.

TSIAPFC			
<u>XXIAPFC</u>	<u>TSIXPXC</u>	<u>TSXXPFC</u>	<u>XSXXPXC</u>
#sequences:	#sequences:	#sequences:	#sequences:
41 (37 unique)	45 (42 unique)	64 (63 unique)	9
APIAPFC	TSIAPNC	TSAEPFC	DSEVPTC
EFIAPFC	TSIAPSC	TSAPPFC	ESADPLC
EGIAPFC	TSIAPVC	TSASPFC	HSTIPLC
FGIAPFC	TSIAPYC	TSAVPFC	QSWGPTC
GAIAPFC	TSIDPIC	TSDGPFPC	TSPYPLC
GEIAPFC	TSIFPWC	TSDLPFC	VSEAPLC
GFIAPFC	TSIGPLC	TSDQPFC	WSNLPQC
GGIAPFC	TSIGPTC	TSEFPFC	YSTIPMC
GIIAPFC	TSIGPVC*	TSEKPFPC	YSTTPLC
GLIAPFC	TSIGPVC*	TSEQPFC	
GPIAPFC	TSIGPYC	TSESPFC	
GVIAPFC	TSIHPLC	TSETPFC	
GYIAPFC	TSIHPVC	TSFLPFC	
HDIAPFC	TSIIPAC	TSFSPFC	
HLIAPFC*	TSILPLC	TSFVPFC	
HLIAPFC*	TSILPSC	TSGSPFC	
HSIAPFC*	TSILPTC	TSHGPFPC	
HSIAPFC*	TSILPWC	TSHPPFC	
ISIAPFC	TSINPWC	TSIHPFC	
LAIAPFC	TSIPPLC	TSIIPFC	
LDIAPFC	TSIPPVC	TSIQPFC	
NLIAPFC	TSIPPYC	TSIRPFC	
NVIAPFC	TSIQPLC	TSISPFC	
NYIAPFC	TSIQPNC	TSKQPFC	
PLIAPFC	TSIQPQC	TSKVPFC	
QLIAPFC	TSISPIC	TSLMPFC	
SDIAPFC	TSISPLC	TSLNPFC	
SNIAPFC*	TSISPNC	TSLPPFC	
SNIAPFC*	TSISPOC	TSLSPFC	
STIAPFC	TSISPTC	TSLVPFC	
SVIAPFC	TSITPLC	TSMEPFC	
SYIAPFC	TSITPMC	TSMTPFC	
TNIAPFC	TSITPQC	TSMYPFC	
TQIAPFC*	TSITPVC	TSNSPFC	
TQIAPFC*	TSIVPAC	TSNVPFC	
VLIAPFC	TSIVPHC	TSQAPFC	
VYIAPFC	TSIVPLC*	TSQDPFC	
WGIAPFC	TSIVPLC*	TSQEPFC	
WSIAPFC	TSIVPVC	TSQGPFC	

YAIAPFC
YQIAPFC

TSIVPWC*
TSIVPWC*
TSIWPLC
TSIWPVC
TSIYPFC
TSIYPSC

TSRDPFC
TSRFPFC
TSRQPFC
TSRSPFC
TSRTPFC
TSRVVFC
TSRYVFC
TSSIPFC
TSSLVFC
TSSSPFC*
TSSSPFC*
TSTFPFC
TSTNPFC
TSTPPFC
TSTSPFC
TSTTPFC
TSVDPFC
TSVMPFC
TSVPPFC
TSVQVFC
TSVRVFC
TSVTVFC
TSVWVFC
TSWNPFC
TSWSPFC

Mutations
accepted(#)

Position 7

A(1)
E(2)
F(1)
G(9)
H(3)
I(1)
L(2)
N(3)
P(1)
Q(1)
S(5)
T(2)
V(2)
W(2)
Y(2)
Position 6
A(3)
D(3)
E(1)
F(2)

Position 4

A(4)
D(1)
F(1)
G(4)
H(2)
I(1)
L(4)
N(1)
P(3)
Q(3)
S(5)
T(4)
V(5)
W(2)
Y(2)
Position 2
A(2)
F(1)
H(1)
I(2)

Position 5

A(4)
D(3)
E(5)
F(3)
G(1)
H(2)
I(5)
K(2)
L(5)
M(3)
N(2)
Q(4)
R(7)
S(3)
T(5)
V(7)
W(2)
Position 4
A(1)
D(3)

Position 7

D(1)
E(1)
H(1)
Q(1)
T(2)
V(1)
W(1)
Y(2)
Position 5
A(1)
E(2)
N(1)
P(1)
T(3)
W(1)
Position 4
A(1)
D(1)
G(1)
I(2)

G(4)
I(1)
L(6)
N(2)
P(2)
Q(2)
S(3)
T(1)
V(3)
Y(4)

L(9)
M(1)
N(3)
Q(3)
S(3)
T(3)
V(7)
W(4)
Y(3)

E(3)
F(3)
G(3)
H(1)
I(2)
K(1)
L(3)
M(2)
N(3)
P(5)
Q(6)
R(2)
S(11)
T(5)
V(6)
W(1)
Y(2)

L(1)
T(1)
V(1)
Y(1)
Position 2
L(5)
M(1)
Q(1)
T(2)

Table S2. Sequences tested but for which products could not be detected. The rules here are: no Cys any position; no Arg/Lys in positions 7,6, or 2; no Asp/Glu/Pro in position 2.

TSIAPFC

XXIAPFC

#sequences:

31

TSIXPXC

#sequences:

23

TSXXPFC

#sequences:

56 (55
unique)

XSXXPXC

#sequences:

56

Follow rules

HHIAPFC

MNIAPFC

MSIAPFC

DIIAPFC

ITIAPFC

NYIAPFC

PIIAPFC

PNIAPFC

QPIAPFC

Break rules

DRIAPFC

VRIAPFC

RPIAPFC

CRIAPFC

RTIAPFC

RRIAPFC

RGIAPFC

REIAPFC

ARIAPFC

TRIAPFC

REIAPFC

IKIAPFC

LKIAPFC

KCIAPFC

SKIAPFC

KHIAPFC

DKIAPFC

KQIAPFC

IKIAPFC

CLIAPFC

CGIAPFC

MCIAPFC

Follow rules

TSIKPFC

TSIRPFC

TSIRPGC

TSIRPLC

TSISPGC

TSIMPGC

TSIDPFC

TSIGPFC

Break rules

TSIPPFC

TSISPFC

TSIHPFC

TSIRPFC

TSIFPFC

TSITPFC

TSILPFC

TSIQPFC

TSIRPFC

TSIGPFC

TSIAPEC

TSIVPFC

TSILPFC

TSILPFC

TSIVPFC

Follow rules

TSGYPFC

TSRKPFC

TSRAPFC

TSRPPFC

TSLRPFC

TSRRPFC

TSRGPFC

TSRHPFC

TSRGPFC

TSRDPFC

TSRHPFC

TSRFPFC

TSRSPFC

TSQRPFC

TSHRPFC

TSMRPFC

TSYRPFC

TSHTPFC

TSHHPFC

TSHPPFC

TSHLPFC

TSHVPFC

TSKVPFC

TSKLPFC

TSKHPFC

TSKFPFC

TSKGPFC

TSTKPFC*

TSTKPFC*

TSLKPFC

TSNKPFC

TSPWPFC

TSPLPFC

TSPIPFC

TSPGPFC

TSPTPFC

TSPSPFC

TSTDPFC

Follow rules

SSENPTC

DSNSPFC

SSMGPFC

ASAHPTC

NSVHPFC

YSFSPFC

NSYEPLC

FSGLPHC

GSNPPFC

GSNYPFC

SSSGPFC

ASGLPFC

WSNNPFC

PSPAPFC

NSPAPFC

Break rules

ESWCPLC

CSALPLC

TSECLFC

KSKMPFC

KSHPPFC

KSLKPFC

ISSKPFC

ISAIPFC

NSDWPFC

TSTKPFC

GSTKPFC

DSFKPLC

NSKPPFC

VSKVPLC

ASEKPLC

RSKVPFC

RSTAPFC

SSRQPTC

WSRHPPC

ASGVPRC

RSPEPFC

TSSDPFC	YRSRPTC
TSNDPFC	ASRTPLC
TSDWPFC	KSLQPRC
TSFEPFC	RSTVPAC
TSFIPFC	MSSRPSC
TSQSPFC	ASRFPGC
TSNMPFC	YSRHPTC
TSGQPFC	ASRRPDC
TSGGPFC	SSGRPVC
	QSSLPGC
<u>Break rules</u>	TSSRPGC
TSRCPFC	YNSSPGC
TSDCPFC	HSSNPEC
TSCDPFC	NSSYPEC
TSCLPFC	GSTNPEC
TSECPFC	TSPGPDC
TSCVPFC	ISDWPPC
TSCGPFC	LSDYPPC
TSVCPFC	WSLAPPC
TSSCPFC	GSYEPPC
TSPCPFC	

Mutations not
found / break
rules (#)

Position 7	Position 4	Position 5	Position 7
A(1)	A(1)	C(4)	A(5)
C(3)	F(1)	D(1)	C(1)
D(2)	G(1)	E(1)	D(1)
I(2)	H(1)	P(1)	E(1)
K(3)	L(3)	R(1)	G(3)
L(1)	M(1)	S(1)	H(1)
M(1)	P(1)	V(1)	I(3)
Q(1)	Q(1)	Position 4	K(4)
R(6)	R(2)	C(6)	M(1)
S(1)	S(1)	D(1)	N(3)
T(1)	T(1)	G(1)	Q(1)
V(1)	V(2)	H(4)	R(4)
Position 6	Position 2	L(1)	S(2)
C(2)	C(5)	V(1)	T(4)
E(2)	D(3)		V(1)
G(2)	E(1)		W(2)
H(1)	P(5)		Y(3)
K(5)	R(2)		Position 5
L(1)			A(2)
P(1)			D(3)
Q(1)			E(2)
R(6)			F(1)
T(1)			G(2)

H(1)
K(4)
L(3)
N(1)
P(2)
R(7)
S(6)
T(5)
W(1)
Y(1)
Position 4
A(2)
C(2)
E(2)
F(1)
G(1)
H(2)
I(1)
K(6)
L(2)
M(1)
N(2)
P(2)
Q(2)
R(4)
S(2)
T(1)
V(4)
W(1)
Y(2)
Position 2
A(2)
D(2)
G(4)
H(2)
I(3)
K(2)
L(5)
M(1)
P(5)
R(2)
S(4)
T(3)
V(1)
W(1)
Y(1)

Mutations not
found /
follow rules

(#)

Position 7	Position 4	Position 5	Position 7
D(1)	D(1)	D(1)	A(2)
H(1)	G(1)	F(2)	D(1)
I(1)	K(1)	G(3)	F(1)
M(2)	M(1)	H(6)	G(2)
N(1)	R(3)	K(5)	N(3)
P(2)	S(1)	L(2)	P(1)
Q(1)	Position 2	M(1)	S(3)
Position 6	G(3)	N(3)	W(1)
H(1)	L(1)	P(6)	Y(1)
I(2)	S(1)	Q(2)	Position 5
N(2)	T(1)	R(11)	A(1)
P(1)	W(2)	S(1)	E(1)
S(1)		T(2)	F(1)
T(1)		Y(1)	G(2)
Y(1)		Position 4	M(1)
		A(1)	N(4)
		D(4)	P(2)
		E(1)	S(1)
		F(2)	V(1)
		G(5)	Y(1)
		H(4)	Position 4
		I(2)	A(2)
		K(4)	E(1)
		L(3)	G(2)
		M(1)	H(2)
		P(2)	L(2)
		Q(1)	N(1)
		R(6)	P(1)
		S(3)	S(2)
		T(2)	Y(1)
		V(2)	Position 2
		W(2)	H(1)
		Y(1)	L(3)
			M(1)
			Q(2)
			S(5)
			T(1)
			W(1)
			Y(1)

Table S3A. Summary of selectivity data. Numbers “a,b,c” indicate: a, the total number of times that amino acid mutation was observed in products; b, the total number of times the amino acid mutation was observed in a sequence that did not lead to an observable product, when the rules were followed; c, the total number of times the amino acid mutation was observed in a sequence that did not lead to an observable product, when the rules were broken. Positions are indicated by numbers in the top row; if only the number is shown, this number results only from the double mutant library. If they are followed by “(all)” this is the quadruple + double mutant libraries combined. For example, for the amino acid in position 7, Ala was observed a total of once in a product, although it was also seen twice in sequences that followed the rules without leading to a product. It was seen six times in this position in rule breaking sequences. In position 6, “na” refers to the fact that the quadruple mutant library was not varied in that position.

pos	7	7(all)	6	6(all)	5	5(all)	4	4(all)	2	2(all)
A	1,0,1	1,2,6	3,0,0	na	4,0,0	5,1,2	5,1,1	6,3,3	2,0,0	2,0,2
C	0,0,3	0,0,4	0,0,2	na	0,0,4	0,0,4	0,0,6	0,0,8	0,0,5	0,0,5
D	0,1,2	1,2,3	3,0,0	na	3,1,1	3,1,4	4,5,1	5,5,1	0,0,3	0,0,5
E	2,0,0	3,0,1	1,0,2	na	5,0,1	7,1,3	3,1,0	3,2,2	0,0,1	0,0,1
F	1,0,0	1,1,0	2,0,0	na	3,2,0	3,3,1	4,2,1	4,2,2	1,0,0	1,0,0
G	9,0,0	9,2,3	4,0,2	na	1,3,0	1,5,2	7,6,2	8,8,3	0,3,0	0,3,4
H	3,1,0	4,1,1	0,1,1	na	2,6,0	2,6,1	3,4,5	3,6,7	1,0,0	1,1,2
I	1,1,2	1,1,5	1,2,0	na	5,0,0	5,0,0	3,2,0	5,2,1	2,0,0	2,0,3
K	0,0,3	0,0,7	0,0,5	na	2,5,0	2,5,4	1,5,0	1,5,6	0,0,0	0,0,2
L	2,0,1	2,0,1	6,0,1	na	5,2,0	5,2,3	7,3,4	8,5,6	9,1,0	14,4,5
M	0,2,1	0,2,2	0,0,0	na	3,1,0	3,2,0	2,2,1	2,2,2	1,0,0	2,1,1
N	3,1,0	3,4,3	2,2,0	na	2,3,0	3,7,1	4,0,0	4,1,2	3,0,0	3,0,0
P	1,2,0	1,3,0	2,1,1	na	0,6,1	1,8,3	8,2,1	8,3,3	0,0,5	0,0,10
Q	1,1,1	2,1,2	2,0,1	na	4,2,0	4,2,0	9,1,1	9,1,3	3,0,0	4,2,0
R	0,0,6	0,0,10	0,0,6	na	7,11,1	7,11,7	2,9,2	2,9,6	0,0,2	0,0,4
S	5,0,1	5,3,3	3,1,0	na	3,1,1	3,2,7	16,4,1	16,6,3	3,1,0	3,6,4
T	2,0,1	4,0,5	1,1,1	na	5,2,0	8,2,5	9,2,1	10,2,2	3,1,0	5,2,3
V	2,0,1	3,0,2	3,0,0	na	7,0,1	7,1,1	11,2,3	12,2,7	7,0,0	7,0,1
W	2,0,0	3,1,2	0,0,0	na	2,0,0	3,0,1	3,2,0	3,2,1	4,2,0	4,3,1
Y	2,0,0	4,1,3	4,1,0	na	0,1,0	0,1,1	4,1,0	5,2,2	3,0,0	3,1,1

Table S3B. Percent success rate for each amino acid. Amino acids behave similarly as groups, within the limitations of the number of sequences screened, where some amino acids co-occur with disfavored amino acids more frequently at random. For example, D occurs in 12 rule-breaking sequences, while E occurs in 9. Some amino acids, such as Asp/Glu or Arg/Lys, share specific forbidden positions, making them similar.

Amino acid	# successful / # appearances	Success rate
A	17/37	46%
I	14/29	48%
L	35/59	59%
V	32/44	73%
N	17/35	49%
Q	21/33	64%
S	30/65	46%
T	28/51	55%
F	11/20	55%
H	10/37	27%
W	13/25	52%
Y	16/30	53%
D	12/32	38%
E	14/26	54%
G	22/54	41%
M	7/19	37%
P	12/45	27%
K	3/37	8%
R	9/62	15%
C	0/23	0%

Table S3C. Percent acceptance of each amino acid at each position, when rules are followed. Note that -1 indicates a forbidden position, while -2 indicates that no sequence encoded the amino acid in that position. These percentages further reinforce the grouping of amino acids by type.

	7	6	5	4	2
A	33.3	100.0	83.3	66.7	100.0
D	50.0	100.0	75.0	50.0	-1.0
E	100.0	100.0	87.5	60.0	-1.0
F	50.0	100.0	50.0	66.7	100.0
G	81.8	100.0	33.3	50.0	0.0
H	80.0	0.0	25.0	33.3	50.0
I	50.0	50.0	100.0	71.4	100.0
K	-1.0	-1.0	28.6	16.7	-1.0
L	100.0	100.0	50.0	61.5	77.8
M	0.0	-2.0	60.0	50.0	66.7
N	42.9	50.0	30.0	80.0	100.0
P	40.0	66.7	11.1	72.7	-1.0
Q	66.7	100.0	66.7	90.0	66.7
R	-1.0	-1.0	38.9	18.2	-1.0
S	62.5	75.0	60.0	72.7	33.3
T	100.0	50.0	80.0	83.3	71.4
V	100.0	100.0	87.5	85.7	100.0
W	75.0	-2.0	100.0	66.7	57.1
Y	80.0	80.0	0.0	85.7	75.0

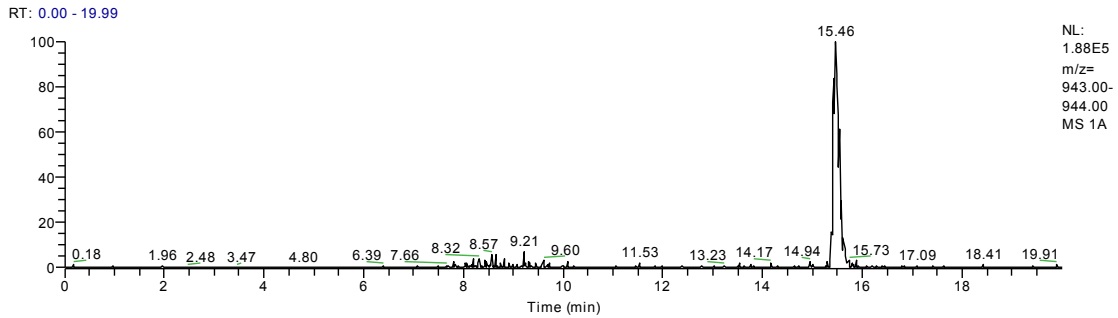
Table S4. Mass spectral analysis of libraries. These represent extracted ion chromatograms for synthesized compounds. The precursor peptide was sequenced, and the sequence was used to generate a table of possible cyanobactin derivatives that might be made. The resulting m/z values were manually sought. When found, adjacent spectra were examined to ensure that the peak was specifically correlated with the compound. Often, two isobaric peaks are present. These are either: 1) regioisomers of isoprenylation; or 2) D and L isomers adjacent to thiazoline. For the second possibility, an identical pattern is seen with the standard, trunkamide. In some cases, the products are not prenylated, while in others products are prenylated as indicated. Finally, isoprene is readily lost by fragmentation, so that searching for the base mass of a compound (without isoprene) often leads to identification of all of the prenylated variants.

S4A. XXIAPFC

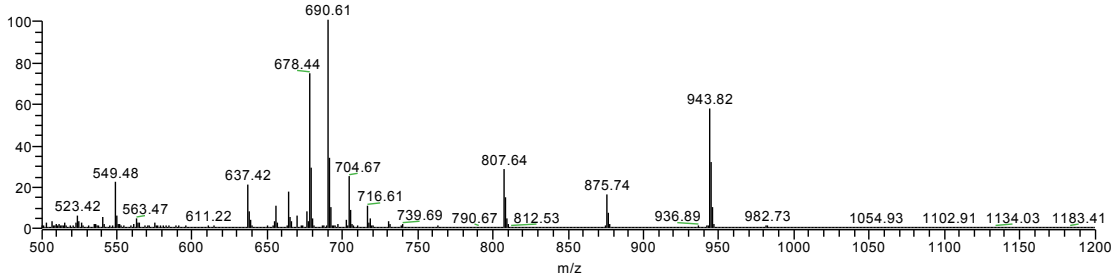
Top: Representative control spectrum for $m/z = 943$, patellin 3 standard. This standard is an internal control that is present in all runs shown below. If patellin 3 is found in an extract, it is highly likely that the new compound will also be found, while if patellin 3 is absent the new compound is universally absent in runs.

F:\Other...\data\XXIAPFC_112311\1A

11/23/2011 1:11:14 PM

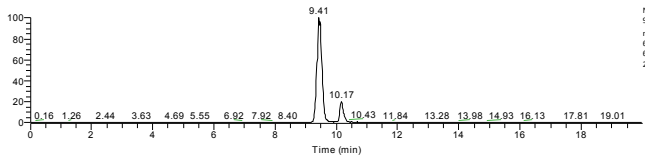
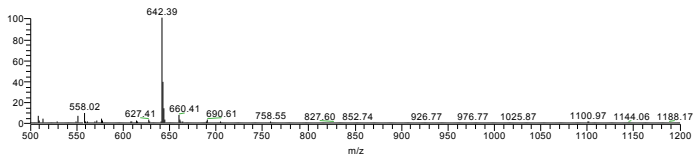
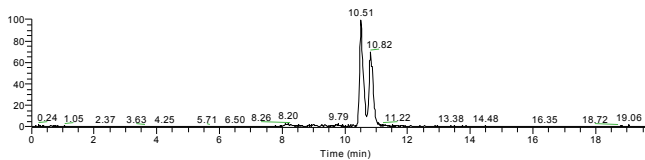
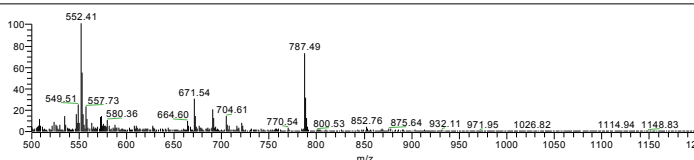
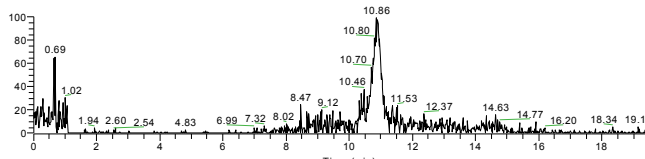
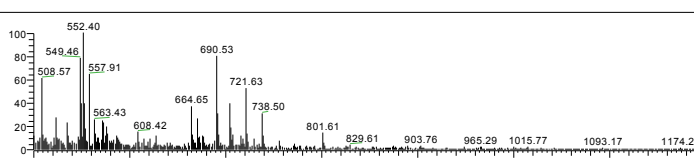
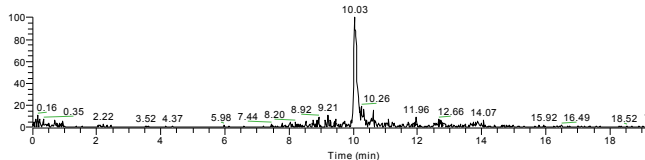
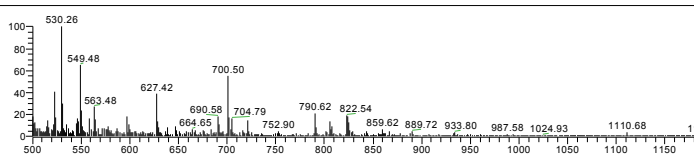


1A #892-908 RT: 15.30-15.58 AV: 17 NL: 1.45E5
T: + c ESI Q1MS [500.000-1200.000]



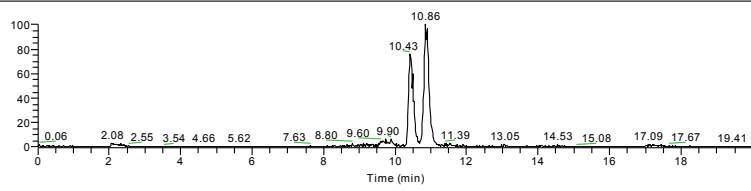
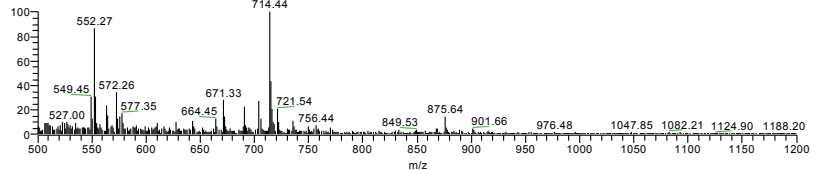
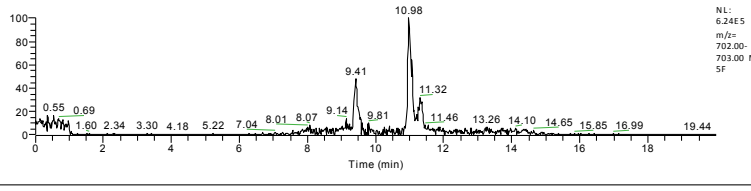
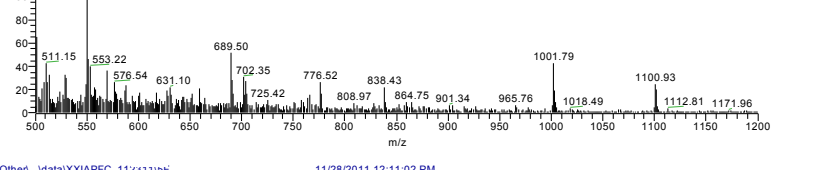
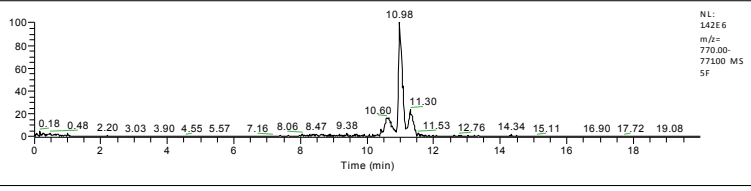
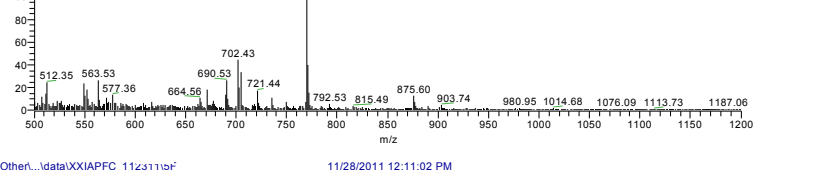
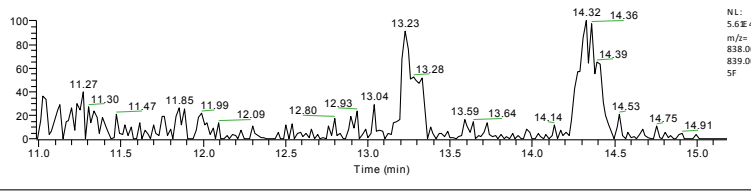
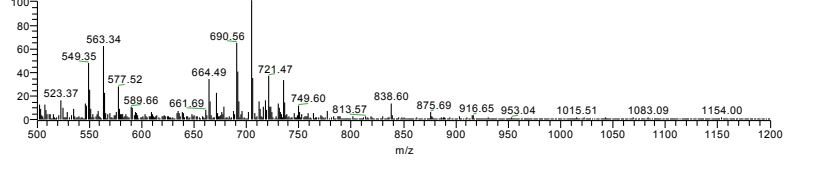
Sequence	m/z	Extracted ion chromatogram and mass spectrum at time point
GPIAPFC	688	<p>F:\Other...\data\XXIAPFC_112311\1A 11/23/2011 1:11:14 PM</p> <p>RT: 0.00 - 19.99</p> <p>10.62</p> <p>NL: 6.93E5 m/z= 668.00-669.00 MS 1A</p> <p>Time (min)</p> <p>1A #606-632 RT: 10.39-10.84 AV: 27 NL: 3.17E5 T: + c ESI Q1MS [500.000-1200.000]</p> <p>688.40</p> <p>m/z</p>

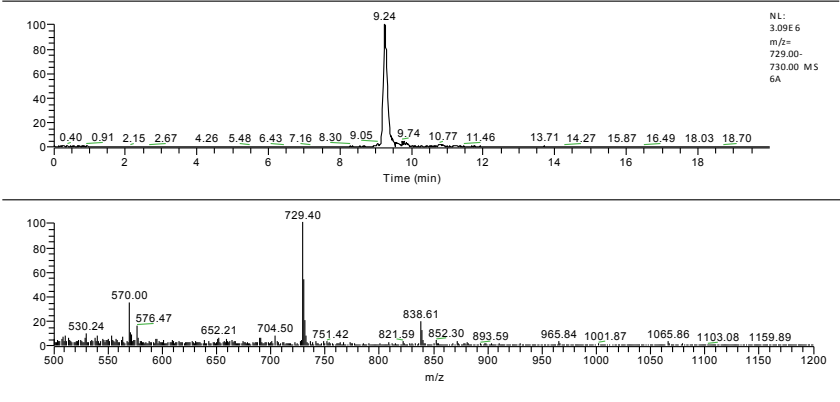
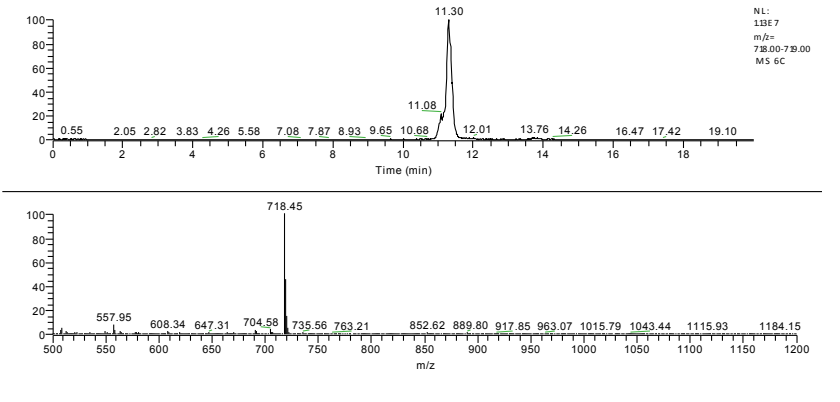
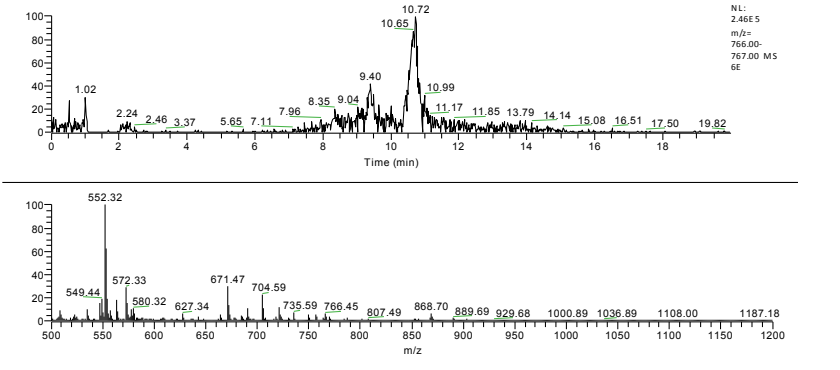
GLIAPFC	684	<p>F:\Other...data\XXIAPFC_11231111U 11/23/2011 2:32:55 PM</p> <p>Chromatogram peaks (min): 0.40, 0.95, 2.15, 3.66, 4.19, 5.12, 7.47, 8.14, 8.25, 8.83, 10.43, 11.18, 11.77, 12.51, 14.17, 15.13, 16.39, 18.29, 18.77</p> <p>Mass spectrum peaks (m/z): 508.19, 547.21, 557.97, 613.36, 664.58, 684.47, 690.63, 704.63, 716.60, 800.53, 868.72, 901.71, 922.09, 1016.82, 1093.09, 1126.24, 1170.28</p> <p>Metadata: NL: 2.36E6, m/z: 684.00, 685.00 MS, 2</p>
TQIAPFC	743	<p>F:\Other...data\XXIAPFC_11231111G 11/23/2011 3:53:58 PM</p> <p>Chromatogram peaks (min): 0.73, 0.68, 2.05, 3.89, 4.54, 6.10, 7.70, 8.01, 8.97, 9.28, 10.22, 10.45, 12.13, 13.79, 15.00, 16.01, 17.13, 18.62, 19.22</p> <p>Mass spectrum peaks (m/z): 513.46, 550.97, 558.16, 627.40, 690.63, 743.50, 781.56, 827.54, 852.75, 926.76, 976.89, 1025.94, 1100.96, 1187.17</p> <p>Metadata: NL: 6.44E5, m/z: 743.00, 744.00 MS, 35</p>
NVIAPFC	727	<p>F:\Other...data\XXIAPFC_11231111H 11/23/2011 4:20:59 PM</p> <p>Chromatogram peaks (min): 0.09, 1.07, 1.39, 3.61, 4.74, 6.08, 7.28, 7.95, 8.47, 8.88, 9.84, 10.05, 10.38, 11.68, 13.86, 14.24, 15.75, 18.07, 19.37</p> <p>Mass spectrum peaks (m/z): 563.04, 601.37, 627.42, 653.20, 727.48, 751.45, 807.65, 855.73, 887.74, 926.66, 990.77, 1026.94, 1125.01, 1189.25</p> <p>Metadata: NL: 5.98E5, m/z: 727.00, 728.00 MS, 24</p>
APIAPFC	682	<p>F:\Other...data\XXIAPFC_11231111A 11/23/2011 4:47:59 PM</p> <p>Chromatogram peaks (min): 0.62, 2.06, 3.61, 4.74, 6.65, 7.66, 7.58, 9.29, 10.05, 10.22, 10.48, 11.13, 12.39, 13.38, 14.62, 16.11, 16.95, 19.50, 19.79, 19.88</p> <p>Mass spectrum peaks (m/z): 629.44, 630.40, 639.43, 646.48, 651.39, 664.54, 671.50, 672.51, 673.55, 682.47, 690.64, 691.65, 704.68, 716.64, 724.67</p> <p>Metadata: NL: 5.67E5, m/z: 682.00, 683.00 MS, 2A</p>

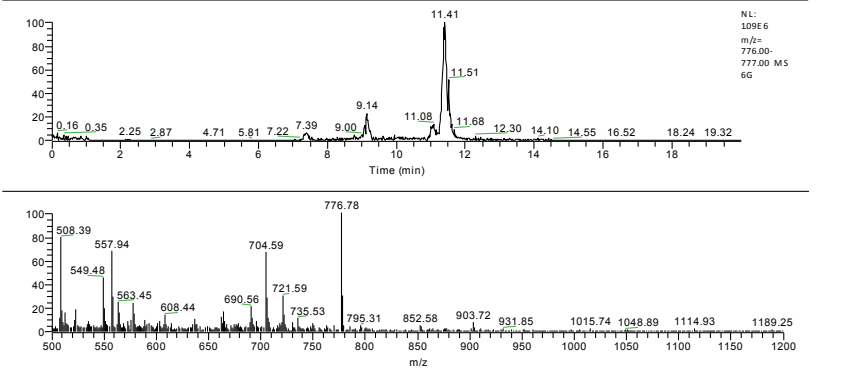
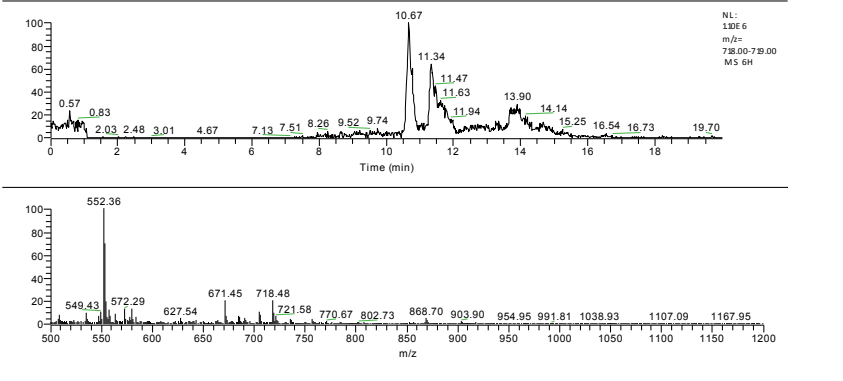
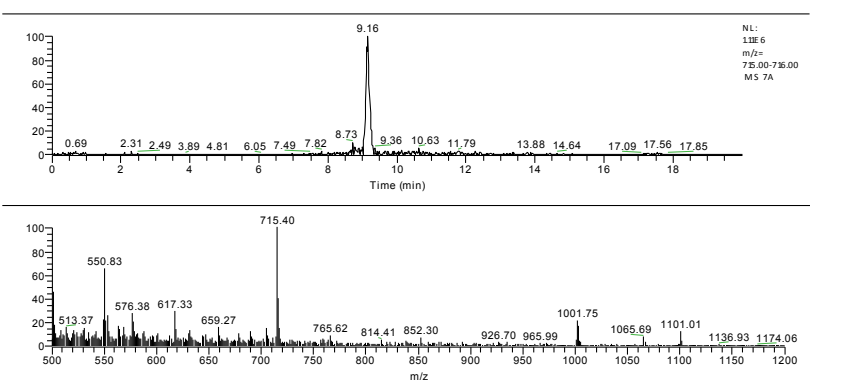
GAIAPFC	642	<p>F:\Other...data\XXIAPFC_112311\z0 11/23/2011 5:42:01 PM</p>  <p>Time (min)</p>  <p>m/z</p> <p>NL: 9.38 E m/z= 642.00- 643.00 MS ZC</p>
WSIAPFC	787	<p>F:\Other...data\XXIAPFC_112311\z0 11/23/2011 6:09:04 PM</p>  <p>Time (min)</p>  <p>m/z</p> <p>NL: 1476.6 m/z= 787.00- 788.00 MS ZC</p>
HSIAPFC	738	<p>F:\Other...data\XXIAPFC_112311\z0 11/23/2011 7:03:06 PM</p>  <p>Time (min)</p>  <p>m/z</p> <p>NL: 1488.5 m/z= 738.00- 739.00 MS ZC</p>
SVIAPFC	700	<p>F:\Other...data\XXIAPFC_112311\z0 11/23/2011 7:30:06 PM</p>  <p>Time (min)</p>  <p>m/z</p> <p>NL: 3.07 E5 m/z= 700.00- 701.00 MS ZC</p>

WGIAPFC	757	<p>F:\Other...data\XXIAPFC_1123113C 11/23/2011 9:18:09 PM</p> <p>Chromatogram Peak: 10.98 min</p> <p>Mass Spectrum Base Peak: 757.50 m/z</p> <p>Other peaks (min): 0.35, 1.07, 2.17, 3.16, 3.76, 5.67, 6.49, 7.80, 8.59, 9.19, 9.96, 11.34, 12.97, 13.62, 15.58, 16.52, 17.78, 19.82</p> <p>Other peaks (m/z): 549.50, 627.42, 664.57, 690.60, 721.59, 784.68, 853.72, 889.66, 915.80, 981.89, 1020.00, 1115.09, 1175.26</p> <p>Metadata: NL: 3.98E 6, m/z: 757.00-758.00 MS, 3C</p>
GEIAPFC	700	<p>F:\Other...data\XXIAPFC_1123113E 11/23/2011 10:12:13 PM</p> <p>Chromatogram Peaks: 9.36, 9.90 min</p> <p>Mass Spectrum Base Peak: 700.43 m/z</p> <p>Other peaks (min): 0.40, 1.07, 2.08, 2.82, 4.43, 5.88, 7.49, 8.09, 8.85, 10.17, 11.70, 12.71, 13.69, 14.55, 16.06, 18.07, 19.60</p> <p>Other peaks (m/z): 550.89, 558.05, 617.37, 659.45, 718.46, 765.54, 838.45, 864.72, 926.74, 972.28, 1001.84, 1065.60, 1100.95, 1188.10</p> <p>Metadata: NL: 1.48E 6, m/z: 700.00-701.00 MS, 3E</p>
EGIAPFC	700	<p>F:\Other...data\XXIAPFC_1123113F 11/23/2011 10:39:13 PM</p> <p>Chromatogram Peak: 9.36 min</p> <p>Mass Spectrum Base Peak: 557.94 m/z</p> <p>Other peaks (min): 0.81, 2.05, 2.24, 3.25, 4.93, 5.62, 6.96, 8.11, 9.12, 10.27, 11.82, 12.61, 13.91, 13.98, 15.96, 16.49, 19.17, 19.65</p> <p>Other peaks (m/z): 530.31, 540.41, 550.90, 553.28, 563.45, 576.36, 577.43, 578.53, 594.33, 609.43, 610.45, 632.59, 643.80, 654.46, 659.40, 668.41, 689.55, 690.58, 700.42, 704.64</p> <p>Metadata: NL: 3.34E 5, m/z: 700.00-701.00 MS, 3F</p>
GGIAPFC	628	<p>F:\Other...data\XXIAPFC_1123113B 11/24/2011 12:27:18 AM</p> <p>Chromatogram Peak: 9.26 min</p> <p>Mass Spectrum Base Peak: 628.34 m/z</p> <p>Other peaks (min): 0.81, 2.37, 2.91, 3.88, 4.93, 6.29, 6.67, 8.23, 8.45, 10.02, 10.93, 10.15, 11.46, 12.23, 13.71, 14.94, 16.54, 17.59, 18.36</p> <p>Other peaks (m/z): 508.40, 540.48, 557.95, 576.39, 684.49, 755.53, 805.59, 838.65, 852.67, 916.20, 965.84, 1008.87, 1065.72, 1114.96, 1180.44</p> <p>Metadata: NL: 1.80E 6, m/z: 628.00-629.00 MS, 4B</p>

GYIAPFC	734	<p>F:\Other...data\XXIAPFC_11231114C 11/24/2011 12:54:18 AM</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 5.92E5 m/z: 734.00- 735.00 MS 4C</p>
LDIAPFC	742	<p>F:\Other...data\XXIAPFC_11231114D 11/24/2011 1:21:20 AM</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 4.40E6 m/z: 742.00- 743.00 MS 4D</p>
SYIAPFC	764	<p>F:\Other...data\XXIAPFC_11231114H 11/24/2011 3:09:24 AM</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 3.36E5 m/z: 764.00- 765.00 MS 4H</p>
LAIAPFC	698	<p>F:\Other...data\XXIAPFC_11231115B 11/28/2011 10:22:59 AM</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 4.02E6 m/z: 698.00- 699.00 MS 5B</p>

<p>ISIAPFC</p>	<p>714</p>	<p>F:\Other...data\XXIAPFC_11231105C 11/28/2011 10:49:59 AM</p>  <p>Time (min)</p>  <p>m/z</p>
<p>STIAPFC</p> <p>+prenyl</p> <p>+2prenyl</p>	<p>702</p> <p>770</p> <p>838</p>	<p>F:\Other...data\XXIAPFC_11231105F 11/28/2011 12:11:02 PM</p>  <p>Time (min)</p>  <p>m/z</p> <p>F:\Other...data\XXIAPFC_11231105F 11/28/2011 12:11:02 PM</p>  <p>Time (min)</p>  <p>m/z</p> <p>F:\Other...data\XXIAPFC_11231105F 11/28/2011 12:11:02 PM</p>  <p>Time (min)</p>  <p>m/z</p>

<p>TNIAPFC</p>	<p>729</p>	<p>F:\Other...data\XXIAPFC_11231116A 11/28/2011 1:32:05 PM</p>  <p>Chromatogram (Time (min)) peaks: 0.40, 0.91, 2.15, 2.67, 4.26, 5.48, 6.43, 7.16, 8.30, 9.05, 9.24, 9.74, 10.77, 11.46, 13.71, 14.27, 15.87, 16.49, 18.03, 18.70</p> <p>Mass Spectrum (m/z) peaks: 530.24, 570.00, 576.47, 652.21, 704.50, 729.40, 751.42, 821.59, 838.61, 852.30, 893.59, 965.84, 1001.87, 1065.86, 1103.08, 1159.89</p> <p>Parameters: NL: 3.09E6, m/z: 729.00-730.00 MS 6A</p>
<p>FGIAPFC</p>	<p>718</p>	<p>F:\Other...data\XXIAPFC_11231116C 11/28/2011 2:26:06 PM</p>  <p>Chromatogram (Time (min)) peaks: 0.55, 2.05, 2.82, 3.83, 4.26, 5.58, 7.08, 7.87, 8.93, 9.65, 10.68, 11.08, 11.30, 12.01, 13.76, 14.26, 16.47, 17.42, 19.10</p> <p>Mass Spectrum (m/z) peaks: 557.95, 608.34, 647.31, 704.58, 718.45, 735.56, 763.21, 852.62, 889.80, 917.85, 963.07, 1015.79, 1043.44, 1115.93, 1184.15</p> <p>Parameters: NL: 1.18E7, m/z: 718.00-719.00 MS 6C</p>
<p>HDIAPFC</p>	<p>766</p>	<p>F:\Other...data\XXIAPFC_11231116E 11/28/2011 3:20:09 PM</p>  <p>Chromatogram (Time (min)) peaks: 1.02, 2.24, 2.46, 3.37, 5.65, 7.11, 7.96, 8.35, 9.04, 9.40, 10.65, 10.72, 10.99, 11.17, 11.85, 13.79, 14.14, 15.08, 16.51, 17.50, 19.82</p> <p>Mass Spectrum (m/z) peaks: 549.44, 552.32, 572.33, 580.32, 627.34, 671.47, 704.59, 735.59, 766.45, 807.49, 868.70, 889.69, 929.68, 1000.89, 1036.89, 1108.00, 1187.18</p> <p>Parameters: NL: 2.46E5, m/z: 766.00-767.00 MS 6E</p>

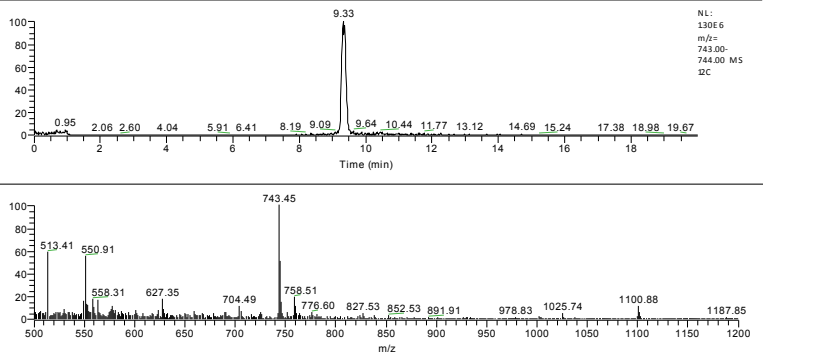
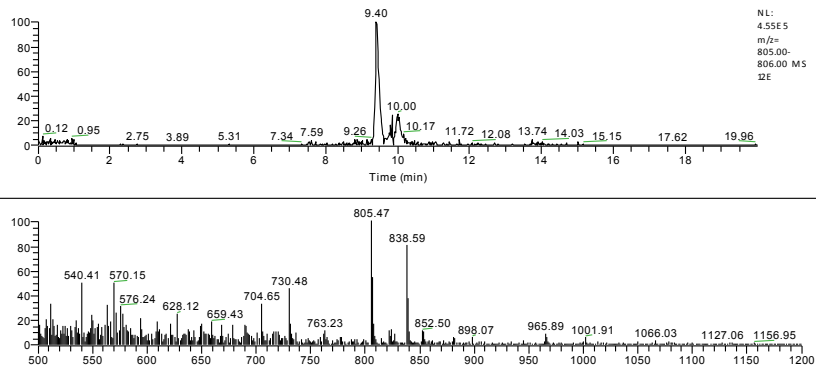
VYIAPFC	776	<p>F:\Other...data\XXIAPFC_11231116G 11/28/2011 4:14:10 PM</p>  <p>Chromatogram peaks (min): 0.16, 0.35, 2.25, 2.87, 4.71, 5.81, 7.22, 7.39, 9.00, 9.14, 11.08, 11.41, 11.51, 11.68, 12.30, 14.10, 14.55, 16.52, 18.24, 19.32</p> <p>Mass spectrum peaks (m/z): 508.39, 549.48, 557.94, 563.45, 608.44, 690.56, 704.59, 721.59, 735.53, 776.78, 795.31, 852.58, 903.72, 931.85, 1015.74, 1048.89, 1114.93, 1189.25</p> <p>Metadata: NL: 109E6, m/z: 776.00, 777.00 MS, 6G</p>
GFIAPFC	718	<p>F:\Other...data\XXIAPFC_11231116H 11/28/2011 4:41:10 PM</p>  <p>Chromatogram peaks (min): 0.57, 0.83, 2.03, 2.48, 3.01, 4.67, 7.13, 7.51, 8.26, 9.52, 9.74, 10.67, 11.34, 11.47, 11.63, 11.94, 13.90, 14.14, 15.25, 16.54, 16.73, 19.70</p> <p>Mass spectrum peaks (m/z): 549.43, 552.36, 572.29, 627.54, 671.45, 718.48, 721.58, 770.67, 802.73, 868.70, 903.90, 954.95, 991.81, 1038.93, 1107.09, 1167.95</p> <p>Metadata: NL: 13E6, m/z: 718.00, 719.00 MS, 6H</p>
SNIAPFC	715	<p>F:\Other...data\XXIAPFC_11231117A 11/28/2011 5:08:12 PM</p>  <p>Chromatogram peaks (min): 0.69, 2.31, 2.49, 3.89, 4.81, 6.05, 7.49, 7.82, 8.73, 9.16, 9.36, 10.63, 11.79, 13.88, 14.64, 17.09, 17.56, 17.85</p> <p>Mass spectrum peaks (m/z): 513.37, 550.83, 576.38, 617.33, 659.27, 715.40, 765.62, 814.41, 852.30, 926.70, 965.99, 1001.75, 1065.69, 1101.01, 1136.93, 1174.06</p> <p>Metadata: NL: 11E6, m/z: 715.00, 716.00 MS, 7A</p>

<p>EFIAPFC</p> <p>790</p>	<p>F:\Other...data\XXIAPFC_11231111\B</p> <p>11/28/2011 5:35:10 PM</p>	<p>Chromatogram peaks (min): 0.69, 1.00, 2.36, 3.44, 4.66, 5.34, 7.58, 8.33, 9.23, 9.62, 9.96, 10.05, 10.12, 10.58, 11.84, 13.72, 13.86, 15.03, 16.95, 17.62, 19.12</p> <p>Mass spectrum peaks (m/z): 530.28, 563.49, 627.35, 704.67, 735.42, 790.57, 868.81, 889.75, 932.69, 986.81, 1049.24, 1108.26, 1138.70</p> <p>Parameters: NL: 1.0E6, m/z: 790.00, 79100 MS, 7B</p>
<p>NYIAPFC</p> <p>791</p>	<p>F:\Other...data\XXIAPFC_11231111\C</p> <p>11/28/2011 9:38:54 PM</p>	<p>Chromatogram peaks (min): 0.95, 1.07, 2.22, 2.49, 3.76, 4.67, 6.67, 7.87, 8.85, 9.00, 9.69, 10.08, 10.15, 10.74, 11.65, 12.52, 13.74, 13.83, 14.00, 15.51, 17.86, 18.50, 19.24</p> <p>Mass spectrum peaks (m/z): 513.35, 550.83, 563.51, 632.45, 690.53, 704.59, 721.56, 791.49, 827.56, 866.64, 926.78, 976.55, 1025.90, 1093.74, 1100.95, 1143.01, 1189.16</p> <p>Parameters: NL: 2.3E5, m/z: 79100, 79200 MS, 8C</p>
<p>GIIAPFC</p> <p>684</p>	<p>F:\Other...data\XXIAPFC_11231111\E</p> <p>11/28/2011 10:32:56 PM</p>	<p>Chromatogram peaks (min): 0.95, 2.12, 2.92, 3.68, 5.33, 6.07, 7.37, 8.28, 8.57, 8.49, 10.53, 11.27, 11.53, 12.35, 14.19, 14.34, 17.23, 18.64, 18.74</p> <p>Mass spectrum peaks (m/z): 547.18, 552.32, 572.33, 580.29, 609.35, 643.36, 671.47, 684.39, 704.65, 770.67, 807.53, 868.72, 903.75, 935.46, 993.70, 1059.47, 1086.84, 1129.93, 1175.22</p> <p>Parameters: NL: 1.1E6, m/z: 684.00, 685.00 MS, 8E</p>

QLIAPFC	755	<p>F:\Other...data\XXIAPFC_112311198 11/29/2011 12:47:59 AM</p>
NLIAPFC	741	<p>F:\Other...data\XXIAPFC_112311198 11/29/2011 2:09:00 AM</p>
YAIAPFC	748	<p>F:\Other...data\XXIAPFC_112311198 11/29/2011 3:30:00 AM</p>

GVIAPFC	670	<p>F:\Other...data\XXIAPFC_11231110B 11/29/2011 9:51:31 AM</p> <p>Chromatogram peaks (min): 0.74, 0.93, 2.17, 3.08, 4.80, 6.34, 7.30, 8.23, 8.52, 9.90, 10.20, 10.26, 10.96, 11.06, 12.42, 13.45, 13.95, 15.68, 17.42, 17.81, 17.90</p> <p>Mass spectrum peaks (m/z): 508.30, 557.88, 563.51, 577.86, 608.31, 670.33, 704.53, 718.58, 749.73, 790.35, 852.56, 882.41, 919.88, 1015.77, 1081.00, 1114.77, 1173.12</p> <p>Parameters: NL: 4.36E5, m/z: 670.00, 671.00 MS, 308</p>
SNIAPFC	715	<p>F:\Other...data\XXIAPFC_11231110C 11/29/2011 10:18:31 AM</p> <p>Chromatogram peaks (min): 0.18, 1.00, 2.30, 3.71, 4.69, 6.08, 7.13, 8.08, 8.95, 9.16, 9.47, 10.36, 11.58, 13.23, 15.24, 16.87, 17.61, 19.82</p> <p>Mass spectrum peaks (m/z): 540.66, 563.31, 617.58, 689.43, 715.32, 730.41, 799.53, 838.52, 885.74, 931.58, 965.80, 989.41, 1079.90, 1139.80, 1186.69</p> <p>Parameters: NL: 2.42E6, m/z: 715.00-716.00, MS, 308</p>
HSIAPFC	738	<p>F:\Other...data\XXIAPFC_11231110E 11/29/2011 11:12:32 AM</p> <p>Chromatogram peaks (min): 0.43, 0.72, 2.10, 2.87, 3.99, 5.00, 6.74, 7.78, 8.52, 9.45, 9.55, 10.51, 10.72, 11.08, 11.97, 12.76, 14.75, 15.41, 17.66, 18.62</p> <p>Mass spectrum peaks (m/z): 508.04, 547.11, 563.41, 571.84, 628.37, 671.46, 704.57, 738.44, 749.59, 807.55, 852.71, 915.37, 952.17, 988.89, 1037.96, 1115.63, 1174.94</p> <p>Parameters: NL: 3.84E5, m/z: 738.00-739.00 MS, 308</p>

SDIAPFC	716	<p>F:\Other...data\XXIAPFC_112311111C 11/29/2011 1:54:35 PM</p> <p>Chromatogram peaks (min): 0.67, 0.72, 2.12, 2.24, 3.56, 4.74, 7.15, 7.92, 8.42, 9.14, 9.47, 11.17, 12.66, 13.76, 13.96, 14.27, 15.22, 16.15, 18.55</p> <p>Mass spectrum peaks (m/z): 511.19, 550.76, 563.39, 576.46, 627.34, 650.33, 704.61, 733.60, 764.73, 852.90, 926.91, 1001.83, 1042.75, 1100.86, 1137.05, 1172.02</p> <p>Parameters: NL: 4.26E5, m/z: 78.00-717.00, MS 1C</p>
PLIAPFC	724	<p>F:\Other...data\XXIAPFC_112311111F 11/29/2011 3:15:38 PM</p> <p>Chromatogram peaks (min): 0.98, 1.07, 2.01, 4.26, 5.83, 7.06, 7.53, 7.71, 8.99, 9.19, 9.33, 9.28, 9.45, 9.62, 9.96, 11.53, 12.71, 14.48, 14.74, 17.14, 18.83</p> <p>Mass spectrum peaks (m/z): 513.37, 530.25, 553.28, 627.37, 659.38, 724.47, 751.46, 758.51, 765.58, 827.60, 877.61, 926.73, 976.70, 1025.89, 1100.96, 1187.19</p> <p>Parameters: NL: 3.08E5, m/z: 724.00-725.00, MS 1F</p>
VLIAPFC	726	<p>F:\Other...data\XXIAPFC_112311111H 11/29/2011 4:09:38 PM</p> <p>Chromatogram peaks (min): 0.18, 0.86, 2.25, 3.39, 3.94, 5.31, 6.60, 7.97, 8.52, 9.09, 9.62, 10.12, 11.92, 12.42, 12.75, 13.98, 14.98, 16.99, 18.38, 19.24</p> <p>Mass spectrum peaks (m/z): 541.01, 563.46, 577.45, 636.18, 690.46, 704.69, 726.53, 735.49, 773.54, 834.90, 903.90, 937.50, 999.45, 1075.12, 1121.74, 1191.30</p> <p>Parameters: NL: 8.29E5, m/z: 726.00-727.00, MS 1H</p>
HLIAPFC	764	<p>F:\Other...data\XXIAPFC_112311112A 11/29/2011 4:36:36 PM</p> <p>Chromatogram peaks (min): 0.74, 0.88, 1.07, 2.19, 2.36, 4.54, 5.00, 5.91, 7.29, 8.13, 8.95, 9.71, 10.31, 11.94, 12.06, 12.23, 12.33, 12.47, 12.73, 13.71, 14.70, 16.49, 17.49, 18.50, 19.51</p> <p>Mass spectrum peaks (m/z): 511.26, 549.44, 563.48, 577.24, 636.60, 690.60, 704.61, 718.68, 764.55, 807.59, 875.75, 853.91, 937.27, 976.92, 1023.74, 1107.04, 1148.16, 1185.09</p> <p>Parameters: NL: 3.38E5, m/z: 764.00-765.00, MS 1A</p>

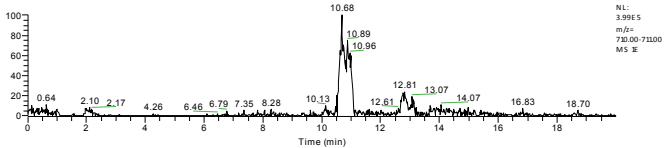
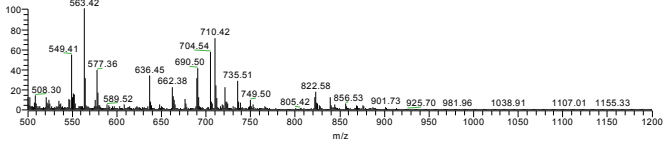
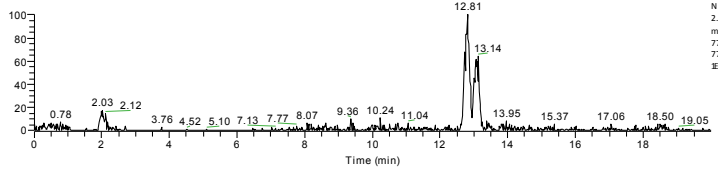
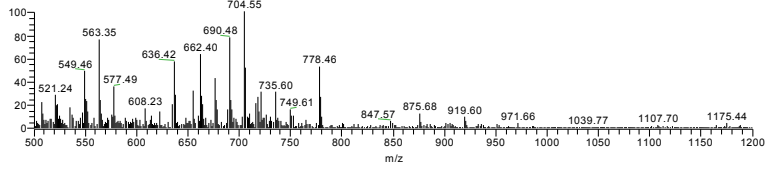
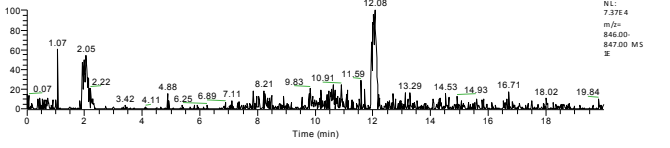
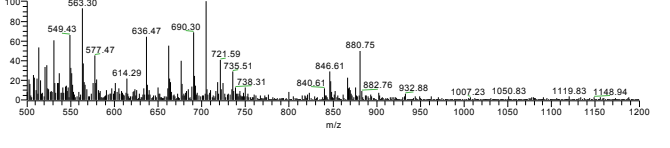
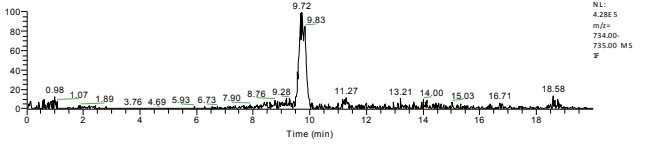
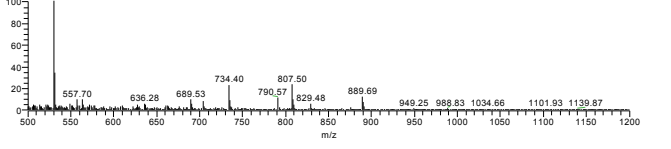
<p>TQIAPFC</p>	<p>743</p>	<p>F:\Other...data\XXIAPFC_112311112C 11/29/2011 5:30:38 PM</p>  <p>Chromatogram (Time in min): 0.95, 2.06, 2.60, 4.04, 5.91, 6.41, 8.19, 9.09, 9.33, 9.64, 10.44, 11.77, 13.12, 14.69, 15.24, 17.38, 18.98, 19.67</p> <p>Mass Spectrum (m/z): 513.41, 550.91, 558.31, 627.35, 704.49, 743.45, 759.51, 776.60, 827.53, 852.53, 891.91, 978.83, 1025.74, 1100.88, 1187.85</p> <p>Parameters: NL: 130E6, m/z: 743.00, 744.00 MS, I2C</p>
<p>YQIAPFC</p>	<p>805</p>	<p>F:\Other...data\XXIAPFC_112311112E 11/29/2011 6:24:39 PM</p>  <p>Chromatogram (Time in min): 0.12, 0.95, 2.75, 3.89, 5.31, 7.34, 7.59, 9.26, 9.40, 10.00, 10.17, 11.72, 12.08, 13.74, 14.03, 15.15, 17.62, 19.96</p> <p>Mass Spectrum (m/z): 540.41, 570.15, 576.24, 628.12, 659.43, 704.65, 730.48, 763.23, 805.47, 838.59, 852.50, 898.07, 965.89, 1001.91, 1066.03, 1127.06, 1156.95</p> <p>Parameters: NL: 4.55E5, m/z: 805.00, 806.00 MS, I2E</p>

S4B. TSIXPXC

Note: An additional complication with this series is that if X is Ser or Thr in position 2 (adjacent to thiazoline), it is readily dehydrated. This dehydration, rather than heterocyclization, was confirmed by MS/MS in previous studies.

Sequence	m/z	Extracted ion chromatogram and mass spectrum at time point
TSIAPNC	669	<p>F:\Other_data\TSIXPXC_1d_9611b 9/19/2011 11:18:41 AM</p> <p>NL: 9.00E6 m/z: 669.00 700.00 MS</p> <p>F:\Other_data\TSIXPXC_1d_9611b 9/19/2011 11:18:41 AM</p> <p>F:\Other_data\TSIXPXC_1d_9611b 9/19/2011 11:18:41 AM</p> <p>NL: 5.53E5 m/z: 737.00 738.00 MS</p> <p>F:\Other_data\TSIXPXC_1d_9611b 9/19/2011 11:18:41 AM</p> <p>F:\Other_data\TSIXPXC_1d_9611b 9/19/2011 11:18:41 AM</p> <p>NL: 1.95E5 m/z: 805.00 806.00 MS</p> <p>F:\Other_data\TSIXPXC_1d_9611b 9/19/2011 11:18:41 AM</p>
+isoprene	737	
+2isoprene	805	

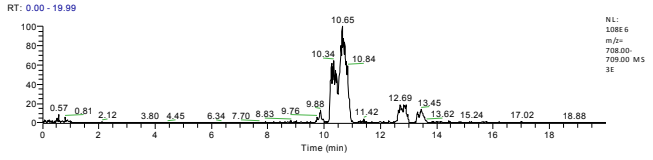
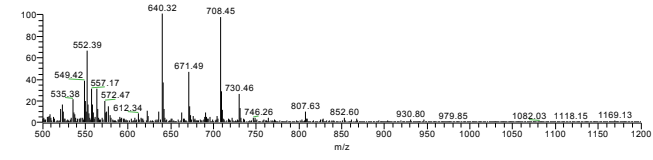
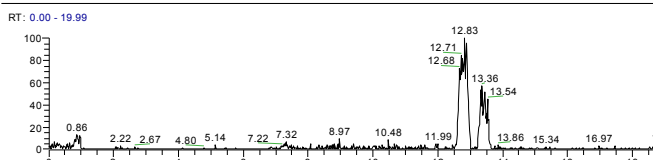
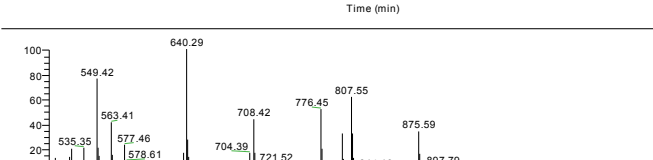
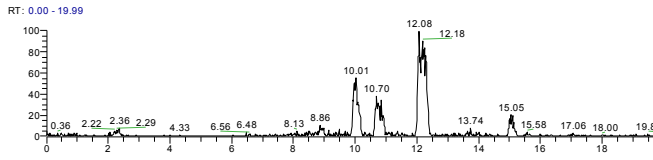
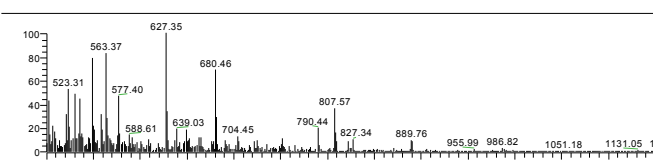

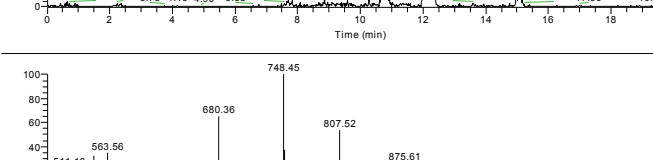
TSIVPHC	720	F:\Other...data\TSIXPXC_1st_9b11C 9/19/2011 11:45:45 AM
+isoprene	788	
+2isoprene	856	
TSIVPHC	769	F:\Other...data\TSIXPXC_1st_9b11C 9/19/2011 11:45:45 AM
+isoprene	837	
TSIVPHC	769	F:\Other...data\TSIXPXC_1st_9b11D 9/19/2011 12:12:45 PM
+isoprene	837	

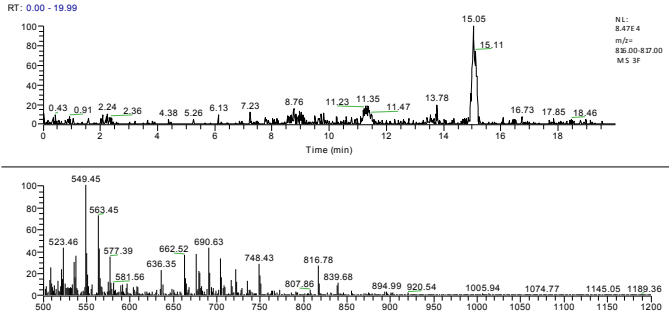
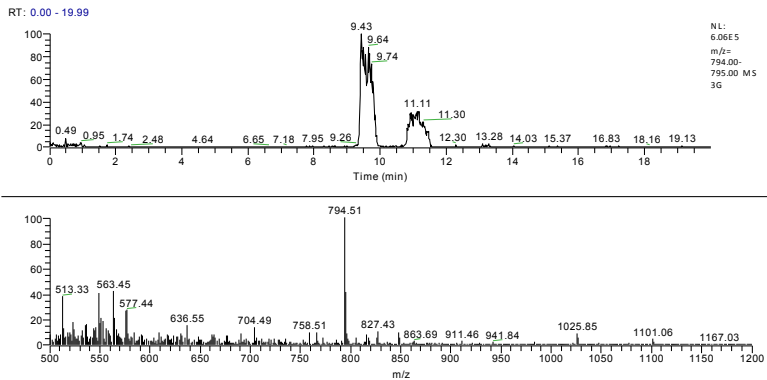
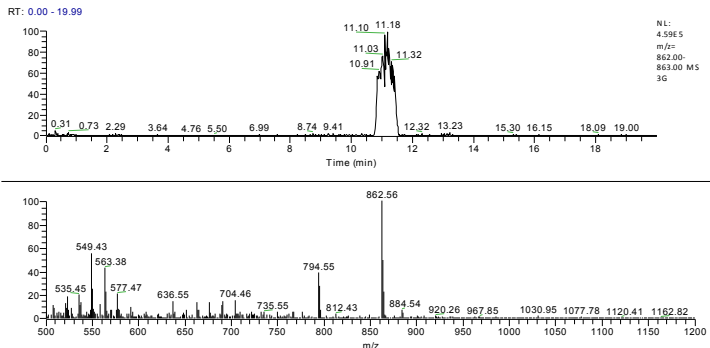
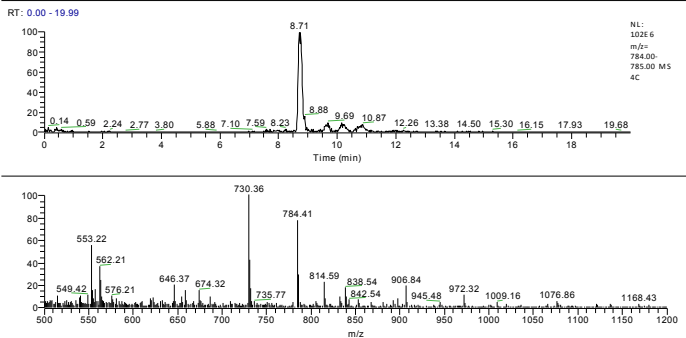
<p>TSILPLC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>710</p> <p>778</p> <p>846</p>	<p>F:\Other_data\TSIXPXC_18_9611E 9/19/2011 12:39:51 PM</p>   <p>F:\Other_data\TSIXPXC_18_9611E 9/19/2011 12:39:51 PM</p>   <p>F:\Other_data\TSIXPXC_18_9611E 9/19/2011 12:39:51 PM</p>  
<p>TSIHPLC</p> <p>+isoprene</p>	<p>734</p> <p>802</p>	<p>F:\Other_data\TSIXPXC_18_9611E 9/19/2011 1:06:53 PM</p> <p>RT: 0.00 - 19.99</p>  

		<p>F:\Other...data\TSIXPXC_1st_9e\117 9/19/2011 1:06:53 PM</p> <p>RT: 0.00 - 19.99</p> <p>11.23 11.29</p> <p>NL: 2.26E5 m/z: 802.00 803.00 MS F</p>
<p>TSISPQC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>699</p> <p>767</p> <p>835</p>	<p>F:\Other...data\TSIXPXC_1st_9e\12 9/19/2011 4:16:13 PM</p> <p>RT: 0.00 - 19.99</p> <p>9.24</p> <p>NL: 3.33E5 m/z: 699.00 700.00 MS 2E</p> <p>F:\Other...data\TSIXPXC_1st_9e\12 9/19/2011 4:16:13 PM</p> <p>RT: 0.00 - 19.99</p> <p>9.23 9.26</p> <p>NL: 5.95E5 m/z: 767.00 768.00 MS 2E</p> <p>F:\Other...data\TSIXPXC_1st_9e\12 9/19/2011 4:16:13 PM</p> <p>RT: 0.00 - 19.99</p> <p>11.06</p> <p>NL: 5.08E4 m/z: 835.00 836.00 MS 2E</p>

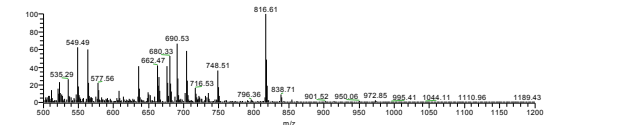
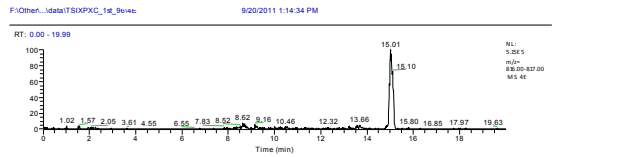
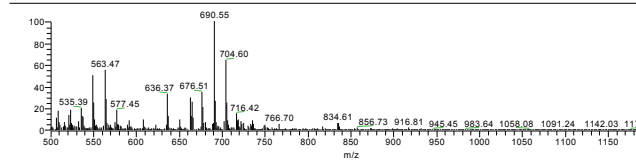
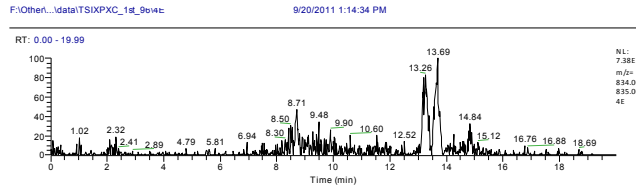
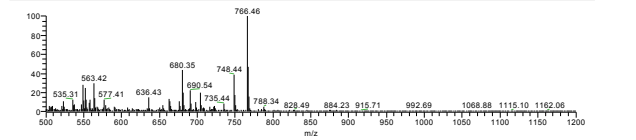
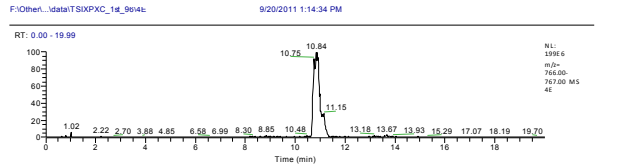
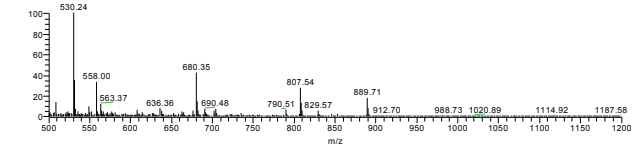
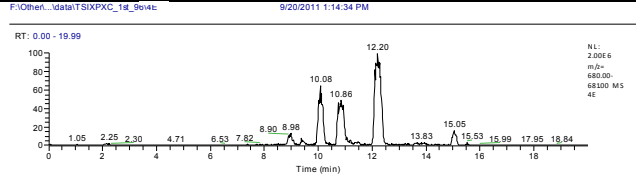
<p>TSIVPLC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>696</p> <p>764</p> <p>832</p>	<p>F:\Other...data\TSIXPXC_1st_9e1us 9/19/2011 6:31:26 PM</p> <p>RT: 0.00 - 19.99</p> <p>10.41, 10.53, 12.68</p> <p>696.39</p> <p>549.35, 597.20, 668.33, 718.55, 749.41, 808.79, 852.46, 889.67, 957.31, 1024.30, 1115.22, 1180.27</p> <p>F:\Other...data\TSIXPXC_1st_9e1us 9/19/2011 6:31:26 PM</p> <p>RT: 0.00 - 19.99</p> <p>12.64, 12.73</p> <p>696.39, 764.55</p> <p>549.42, 597.21, 668.42, 698.53, 704.43, 786.50, 808.72, 876.39, 903.41, 952.62, 1021.64, 1102.14, 1142.32, 1170.25</p> <p>F:\Other...data\TSIXPXC_1st_9e1us 9/19/2011 6:31:26 PM</p> <p>RT: 0.00 - 19.99</p> <p>8.64, 16.81, 16.95</p> <p>663.42</p> <p>1.07, 2.27, 2.20, 3.59, 6.10, 6.51, 7.83, 8.43, 8.49, 8.93, 9.73, 10.62, 11.65, 12.76, 13.02, 14.94, 16.81, 18.89, 18.98</p> <p>663.42, 615.33, 577.43, 636.39, 676.65, 704.42, 743.72, 771.00, 832.78, 854.68, 871.45, 943.95, 1007.29, 1039.92, 1123.42, 1163.32</p>
<p>TSIGPVC</p> <p>+isoprene</p>	<p>640</p> <p>708</p>	<p>F:\Other...data\TSIXPXC_1st_9e1us 9/19/2011 6:58:30 PM</p> <p>RT: 0.00 - 19.99</p> <p>10.26, 10.68, 13.50</p> <p>640.29, 730.43</p> <p>0.40, 2.13, 2.55, 4.69, 5.36, 6.08, 7.02, 8.19, 8.56, 8.88, 9.07, 11.42, 13.33, 13.62, 14.81, 17.37, 18.07, 19.41</p> <p>640.29, 553.28, 562.21, 549.25, 578.39, 662.39, 716.35, 780.98, 838.69, 880.59, 939.04, 965.83, 1019.76, 1076.60, 1121.66, 1176.83</p>

		<p>F:\Other...data\TSIXPXC_1st_8e1a.d</p> <p>9/19/2011 6:58:30 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p>
TSIWPLC	783	<p>F:\Other...data\TSIXPXC_1st_8e1a.d</p> <p>9/19/2011 7:25:32 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p>
+isoprene	851	<p>F:\Other...data\TSIXPXC_1st_8e1a.d</p> <p>9/19/2011 7:25:32 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p>
TSIGPVC	640	<p>F:\Other...data\TSIXPXC_1st_8e1a.d</p> <p>9/19/2011 7:52:35 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p>
+isoprene	708	
+2isoprene	776	

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<p>TSIPPVC +isoprene +2isoprene</p>	<p>680 748 816</p>	<p>F:\Other...data\TSIXPXC_1d_9e\4d 9/19/2011 8:19:39 PM</p>   <p>F:\Other...data\TSIXPXC_1d_9e\4d 9/19/2011 8:19:39 PM</p>  

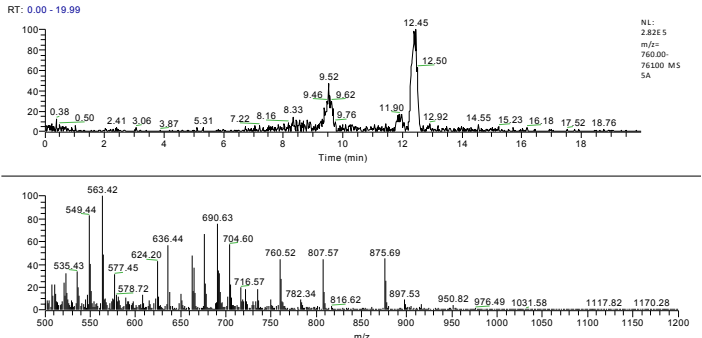
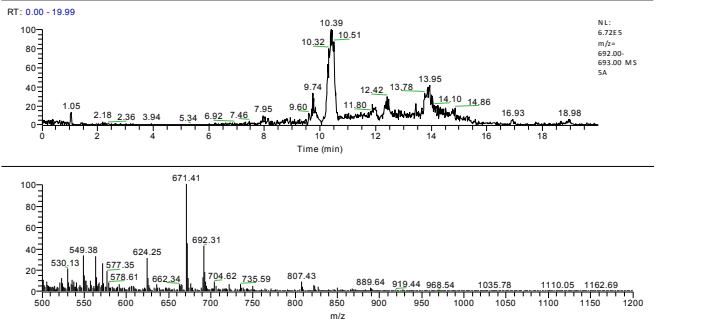
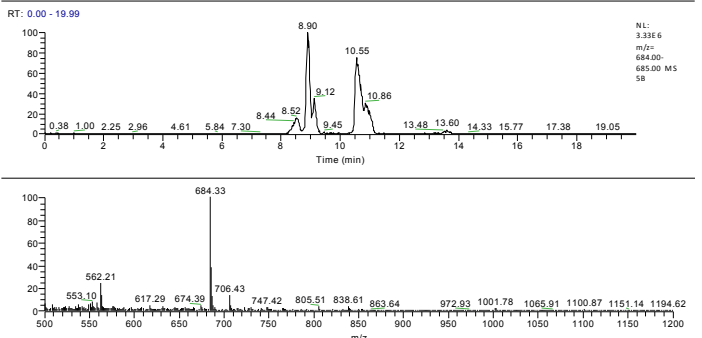
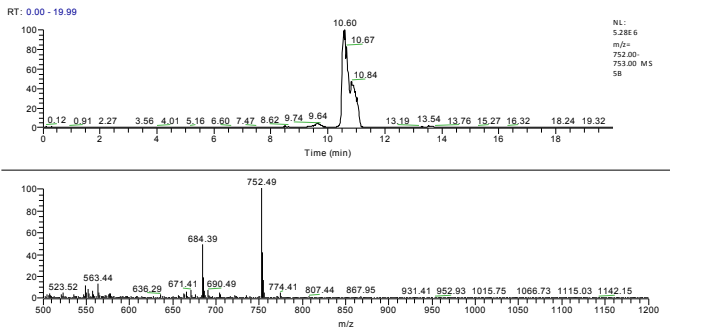
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<p>TSIYPFC +isoprene</p>	<p>794 862</p>	<p>F:\Other...data\TSIXPXC_1st_90v3r 9/19/2011 8:46:39 PM</p>  <p>RT: 0.00 - 19.99</p> <p>9.43</p> <p>9.64</p> <p>9.74</p> <p>11.11</p> <p>11.30</p> <p>NL: 6.06E5 m/z= 794.00 795.00 MS 3G</p> <p>Time (min)</p> <p>794.51</p> <p>513.33</p> <p>563.45</p> <p>577.44</p> <p>636.55</p> <p>704.49</p> <p>758.51</p> <p>827.43</p> <p>863.69</p> <p>911.46</p> <p>941.84</p> <p>1025.85</p> <p>1101.06</p> <p>1167.03</p> <p>m/z</p> <p>F:\Other...data\TSIXPXC_1st_90v3r 9/19/2011 8:46:39 PM</p>  <p>RT: 0.00 - 19.99</p> <p>11.10</p> <p>11.18</p> <p>11.03</p> <p>10.91</p> <p>11.32</p> <p>NL: 4.59E5 m/z= 862.00 863.00 MS 3G</p> <p>Time (min)</p> <p>862.56</p> <p>549.43</p> <p>563.38</p> <p>535.45</p> <p>577.47</p> <p>636.55</p> <p>704.46</p> <p>735.55</p> <p>794.55</p> <p>812.43</p> <p>884.54</p> <p>920.26</p> <p>967.85</p> <p>1030.95</p> <p>1077.78</p> <p>1120.41</p> <p>1162.82</p> <p>m/z</p>
<p>TSINPWC +isoprene</p>	<p>784 852</p>	<p>F:\Other...data\TSIXPXC_1st_90v3r 9/20/2011 12:20:29 PM</p>  <p>RT: 0.00 - 19.99</p> <p>8.71</p> <p>8.88</p> <p>9.69</p> <p>10.87</p> <p>12.26</p> <p>13.38</p> <p>14.50</p> <p>15.30</p> <p>16.15</p> <p>17.93</p> <p>19.68</p> <p>NL: 1.02E6 m/z= 784.00 785.00 MS 4C</p> <p>Time (min)</p> <p>730.36</p> <p>784.41</p> <p>553.22</p> <p>562.21</p> <p>549.42</p> <p>576.21</p> <p>646.37</p> <p>674.32</p> <p>735.77</p> <p>814.59</p> <p>838.54</p> <p>842.54</p> <p>906.84</p> <p>945.48</p> <p>972.32</p> <p>1009.16</p> <p>1076.86</p> <p>1168.43</p> <p>m/z</p>

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TSISPLC	649	<p>F:\Other...data\TSIXPXC_1d_9e4u 9/20/2011 12:47:31 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 2986 m/z: 684.00 685.00 MS 4D</p>
+isoprene	752	<p>F:\Other...data\TSIXPXC_1d_9e4u 9/20/2011 12:47:31 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 5336 m/z: 752.00 753.00 MS 4D</p>
TSILPTC	698	<p>F:\Other...data\TSIXPXC_1d_9e4u 9/20/2011 11:14:34 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 457E5 m/z: 698.00 699.00 MS 4E</p>
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+isoprene	766	
+2isoprene	834	
dht+ipr	748	
dht+2ipr	816	



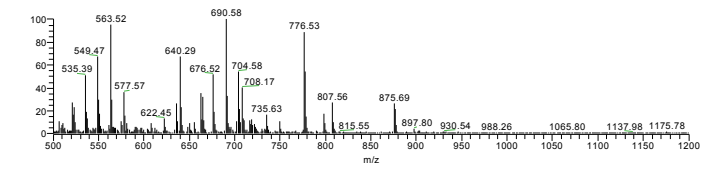
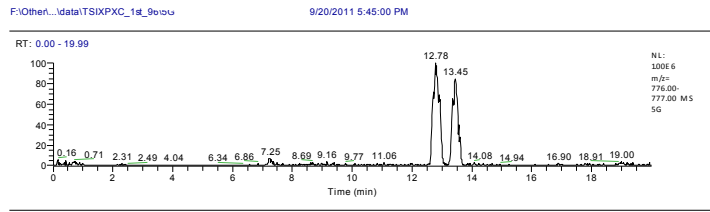
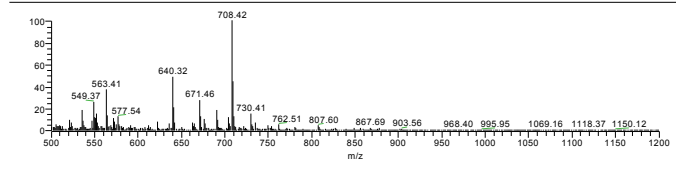
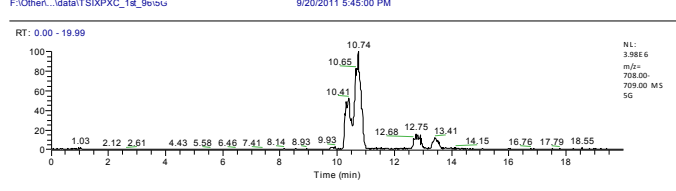
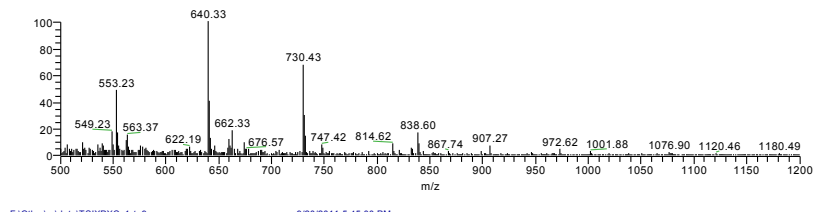
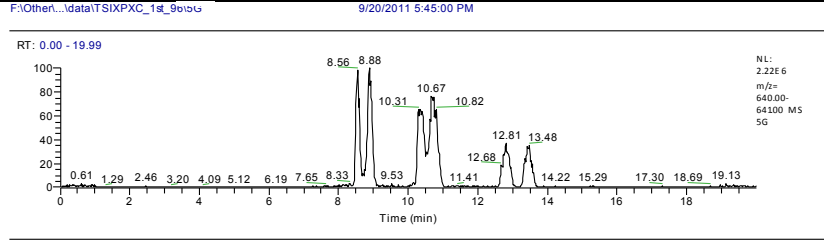
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<p>TSIGPLC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>654</p> <p>722</p> <p>790</p>	<p>F:\Other...data\TSIXPXC_1st_9e14G 9/20/2011 2:08:40 PM</p> <p>RT: 0.00 - 19.99</p> <p>8.97 9.31 10.89 11.20</p> <p>0.86 1.53 2.32 3.32 4.16 5.21 7.03 7.78 7.90 9.65 13.21 13.42 13.59 14.60 16.54 17.88 18.89</p> <p>Time (min)</p> <p>654.33</p> <p>676.22</p> <p>550.84 589.35 631.43 694.25 758.49 800.47 852.67 877.36 942.76 1003.66 1059.31 1100.91 1153.94</p> <p>m/z</p> <p>NL: 244E.6 m/z: 654.00 655.00 MS 4G</p> <p>F:\Other...data\TSIXPXC_1st_9e14G 9/20/2011 2:08:40 PM</p> <p>RT: 0.00 - 19.99</p> <p>10.75 10.87 11.18 11.25</p> <p>1.05 2.12 2.55 3.94 5.79 6.72 7.46 8.06 8.56 10.55 13.21 13.36 13.59 14.62 16.92 18.26 18.82</p> <p>Time (min)</p> <p>722.41</p> <p>654.32</p> <p>549.42 535.40 577.49 636.36 672.35 740.50 744.39 785.28 882.74 958.36 1009.66 1079.11 1116.75 1153.02</p> <p>m/z</p> <p>NL: 287E.6 m/z: 722.00 723.00 MS 4G</p> <p>F:\Other...data\TSIXPXC_1st_9e14G 9/20/2011 2:08:40 PM</p> <p>RT: 0.00 - 19.99</p> <p>9.72 9.88 13.24 13.42 13.62 13.77</p> <p>0.26 1.55 1.46 3.16 4.85 5.65 6.44 7.95 8.81 9.57 11.34 12.14 13.95 14.98 15.67 17.93 18.77</p> <p>Time (min)</p> <p>690.56</p> <p>676.48</p> <p>549.53 535.37 577.48 608.41 662.50 722.48 749.56 790.67 812.59 880.91 917.95 985.76 1072.45 1116.13 1155.26</p> <p>m/z</p> <p>NL: 442E.5 m/z: 790.00 791.00 MS 4G</p>

TSIGPTC	642	F:\Other...data\TSIXPXC_1a_9e1a	9/20/2011 3:02:46 PM
(dehydroT)	624	RT: 0.00 - 19.99	
+isoprene	710		NL: 3.49E5 m/z = 642.00 643.00 MS SA
+2isoprene	778	F:\Other...data\TSIXPXC_1a_9e1a	9/20/2011 3:02:46 PM
dht+ipr	692	RT: 0.00 - 19.99	
dht+2ipr	760		NL: 4.94E5 m/z = 624.00 625.00 MS SA
		F:\Other...data\TSIXPXC_1a_9e1a	9/20/2011 3:02:46 PM
		RT: 0.00 - 19.99	
			NL: 5.76E5 m/z = 725.00 720.00 MS SA
		F:\Other...data\TSIXPXC_1a_9e1a	9/20/2011 3:02:46 PM
		RT: 0.00 - 19.99	
			NL: 2.49E5 m/z = 778.00 779.00 MS SA

		<p>F:\Other...data\TSIXPXC_1st_9e\5A 9/20/2011 3:02:46 PM</p>  <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>563.42, 549.44, 636.44, 690.63, 704.60, 760.52, 807.57, 875.69</p> <p>m/z</p> <p>F:\Other...data\TSIXPXC_1st_9e\5A 9/20/2011 3:02:46 PM</p>  <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>671.41, 549.38, 624.25, 692.31, 704.62, 735.59, 807.43</p> <p>m/z</p>
<p>TSISPIC +isoprene</p>	<p>684 752</p>	<p>F:\Other...data\TSIXPXC_1st_9e\5B 9/20/2011 3:29:49 PM</p>  <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>684.33, 562.21, 706.43, 747.42, 805.51, 838.61</p> <p>m/z</p> <p>F:\Other...data\TSIXPXC_1st_9e\5B 9/20/2011 3:29:49 PM</p>  <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>752.49, 684.39, 690.49, 774.41, 807.44, 867.95</p> <p>m/z</p>

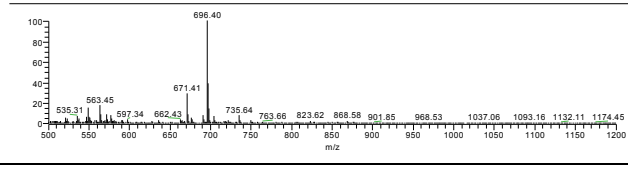
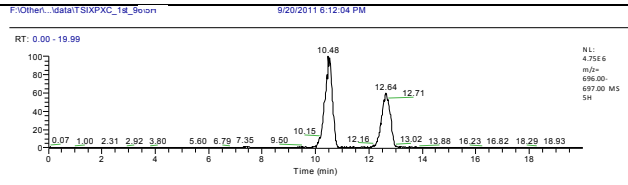
TSIGPVC
 +isoprene
 +2isoprene

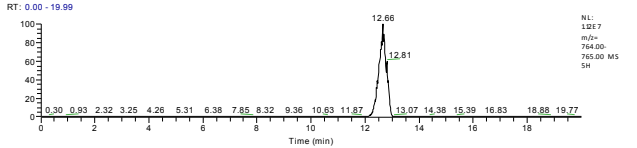
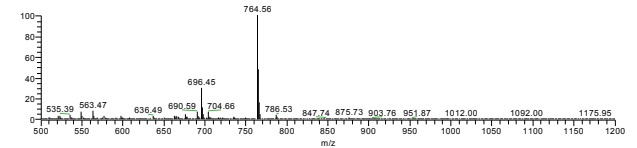
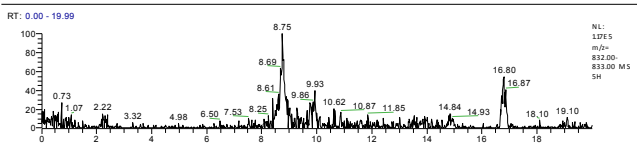
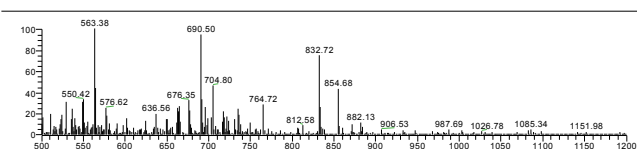
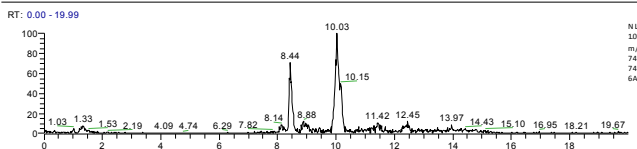
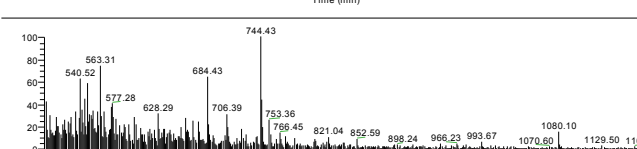
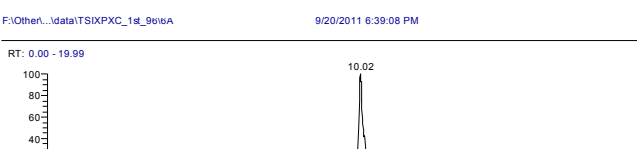
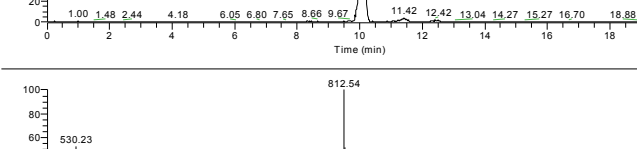
640
 708
 776



TSIVPLC
 +isoprene
 +2isoprene

696
 764
 832

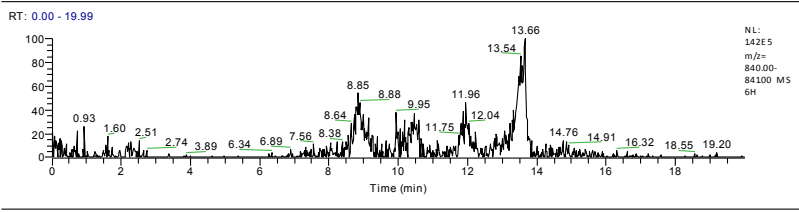
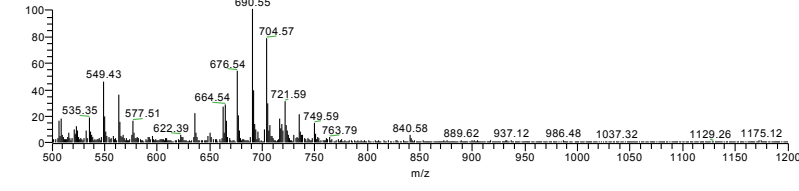
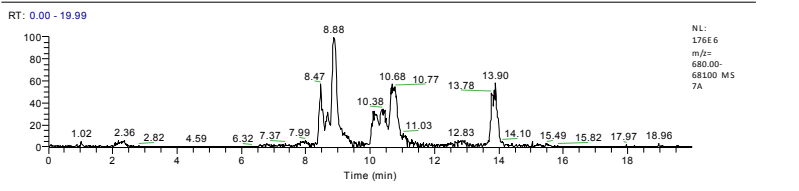
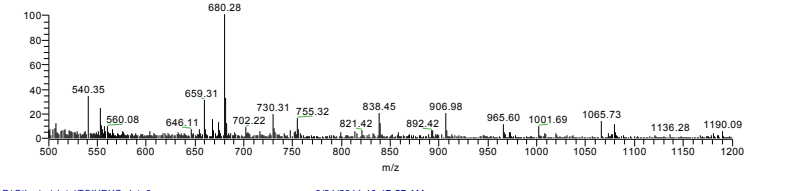
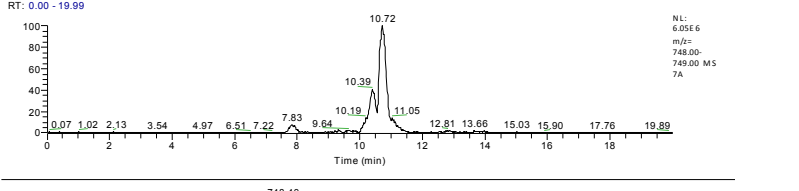
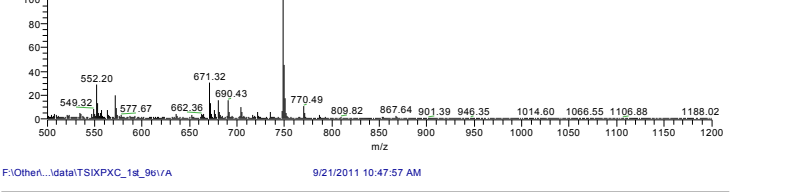
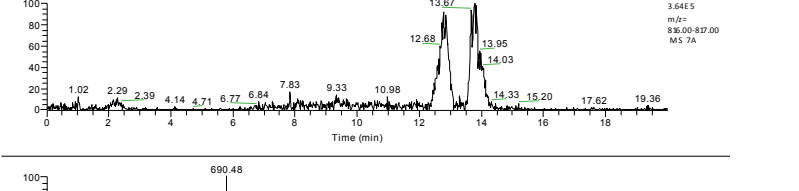
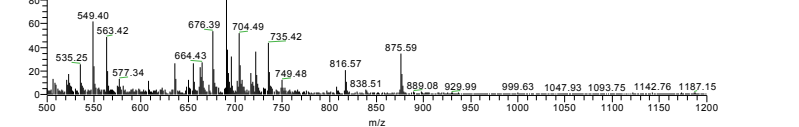


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<p>TSIPPYC +isoprene +2isoprene</p>	<p>744 812 880</p>	<p>F:\Other...data\TSIXPXC_1a_9e3a 9/20/2011 6:39:08 PM</p>   <p>F:\Other...data\TSIXPXC_1a_9e3a 9/20/2011 6:39:08 PM</p>  

		<p>F:\Other...data\TSIXPXC_1st_9@v6A 9/20/2011 6:39:08 PM</p> <p>RT: 0.00 - 19.99</p> <p>NL: 185E5 m/z: 880.00 88100 MS 6A</p>
TSIVPWC +isoprene	769 837	<p>F:\Other...data\TSIXPXC_1st_9@v6U 9/20/2011 8:00:16 PM</p> <p>RT: 0.00 - 19.99</p> <p>NL: 3.96E5 m/z: 769.00 770.00 MS 6D</p> <p>F:\Other...data\TSIXPXC_1st_9@v6U 9/20/2011 8:00:16 PM</p> <p>RT: 0.00 - 19.99</p> <p>NL: 4.66E5 m/z: 837.00 838.00 MS 6D</p>
TSIGPYC +isoprene +2isoprene	704 772 840	<p>F:\Other...data\TSIXPXC_1st_9@v6e 9/20/2011 8:27:19 PM</p> <p>RT: 0.00 - 19.99</p> <p>NL: 4.8E6 m/z: 704.00 705.00 MS 6E</p>

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<p>TSIPPLC +isoprene</p>	<p>762</p>	<p>F:\Other...data\TSIXPXC_1st_9e0e2 9/20/2011 8:27:19 PM</p> <p>RT: 0.00 - 19.99</p> <p>11.06 11.17</p> <p>NL: 1.38E5 m/z= 782.00 783.00 MS 6E</p> <p>721.56 722.54 723.56 730.62 735.57 736.59 743.65 749.69 750.66 756.37 762.49 763.52 770.58 775.68 778.55 785.66 790.48 791.44</p>
<p>TSIDPIC +isoprene +2isoprene</p>	<p>712 780 848</p>	<p>F:\Other...data\TSIXPXC_1st_9e0e2 9/20/2011 9:21:23 PM</p> <p>RT: 0.00 - 19.99</p> <p>10.50 10.39 10.65 10.70</p> <p>NL: 4.35E5 m/z= 730.00-730.00 MS 9E</p> <p>540.10 553.31 576.38 636.15 659.36 671.29 712.34 727.44 838.54 821.43 885.60 907.10 965.62 1001.77 1066.15 1112.76 1180.10</p>

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<p>TSIGPYC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>704</p> <p>772</p> <p>840</p>	<p>F:\Other...data\TSIXPXC_1st_9e1e1H 9/20/2011 9:48:27 PM</p> <p>13.91</p> <p>13.76 14.03 14.10 14.63 15.06 15.53 16.99 18.98</p> <p>0.21 1.02 1.57 2.20 3.47 4.85 6.20 7.99 8.78 8.87 10.84 10.87 11.17 12.71 13.50 13.91 14.03 14.10 14.63 15.06 15.53 16.99 18.98</p> <p>Time (min)</p> <p>NL: 2.63E6 m/z: 704.00-705.00 MS 6H</p> <p>730.40</p> <p>540.17 553.24 576.33 619.09 659.33 704.35 747.57 821.50 838.60 881.22 907.11 917.45 972.99 1001.63 1065.88 1121.37 1180.34</p> <p>m/z</p> <p>F:\Other...data\TSIXPXC_1st_9e1e1H 9/20/2011 9:48:27 PM</p> <p>RT: 0.00 - 19.99</p> <p>11.13</p> <p>11.46 13.59 14.86 15.56 16.99 18.19 19.20</p> <p>0.19 1.00 2.48 3.77 4.92 5.81 6.70 7.27 8.54 9.33 9.90 11.13 11.46 13.59 14.86 15.56 16.99 18.19 19.20</p> <p>Time (min)</p> <p>NL: 6.79E6 m/z: 772.00-773.00 MS 6H</p> <p>772.47</p> <p>549.42 577.63 636.45 690.56 704.46 721.53 772.47 790.45 824.70 889.58 919.65 981.28 1061.97 1157.26 1187.31</p> <p>m/z</p>

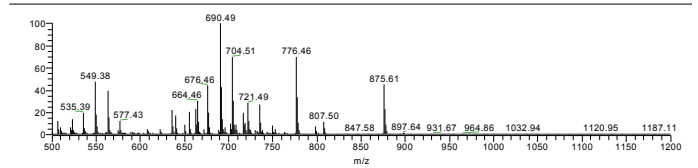
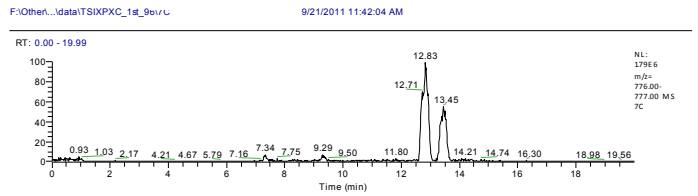
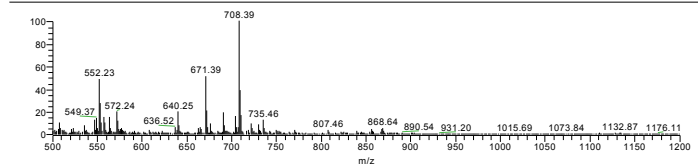
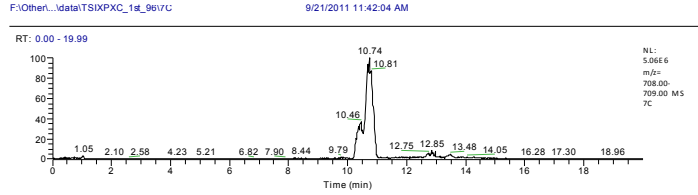
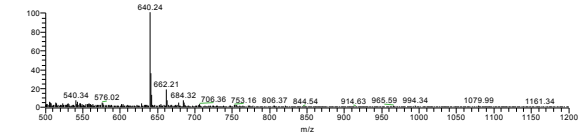
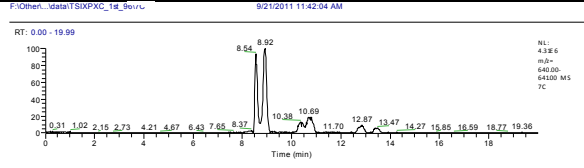
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TSIGPVC
 +isoprene
 +2isoprene

640

708

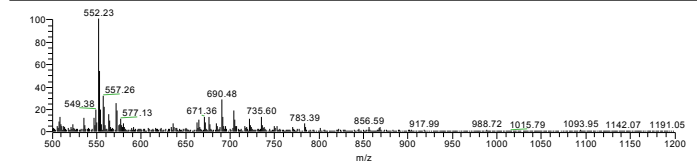
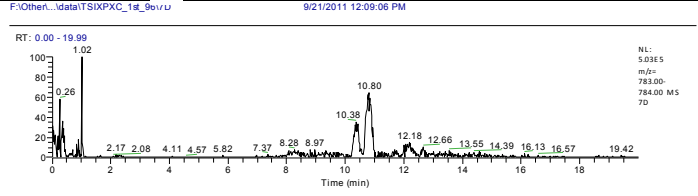
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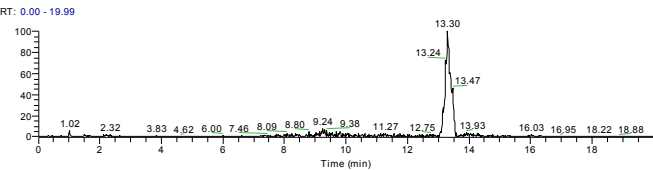
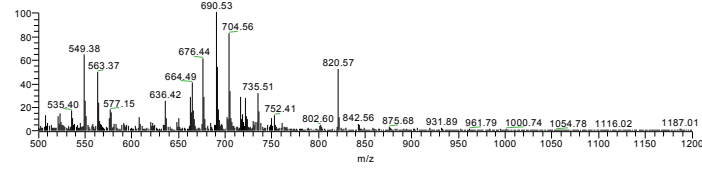
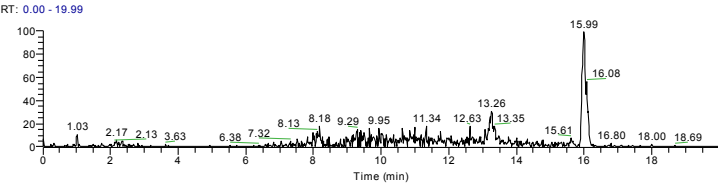
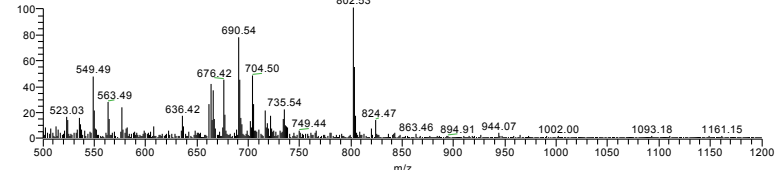
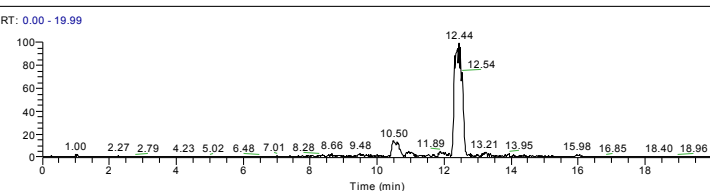
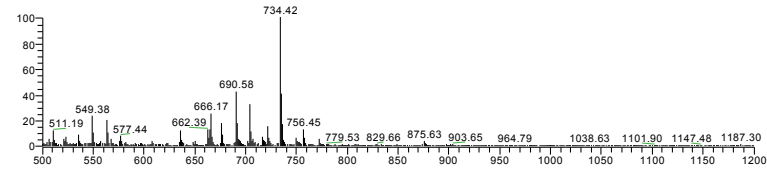
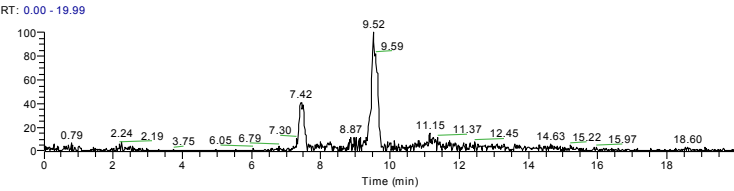
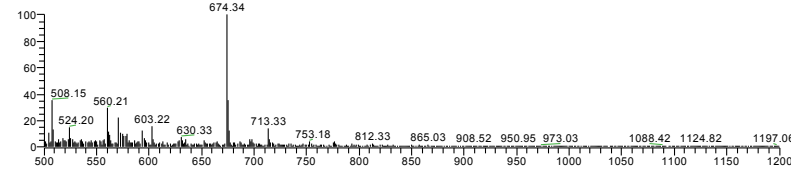
TSILPWC
 +isoprene

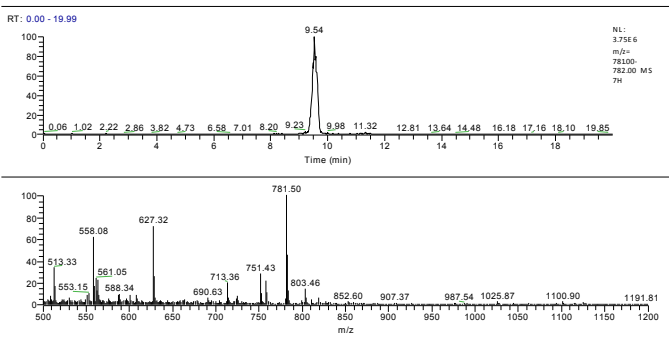
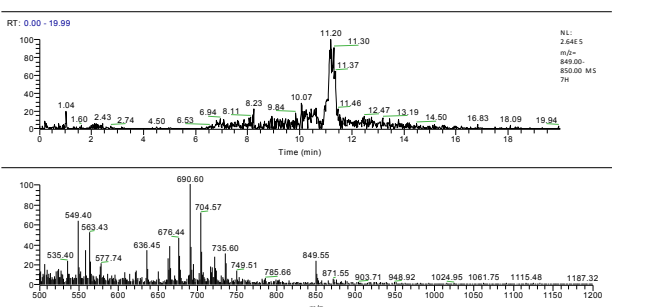
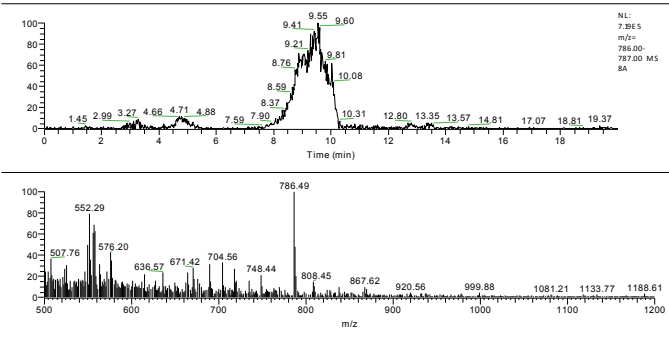
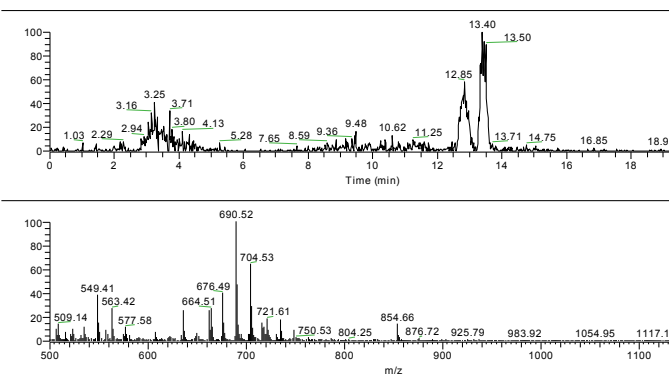
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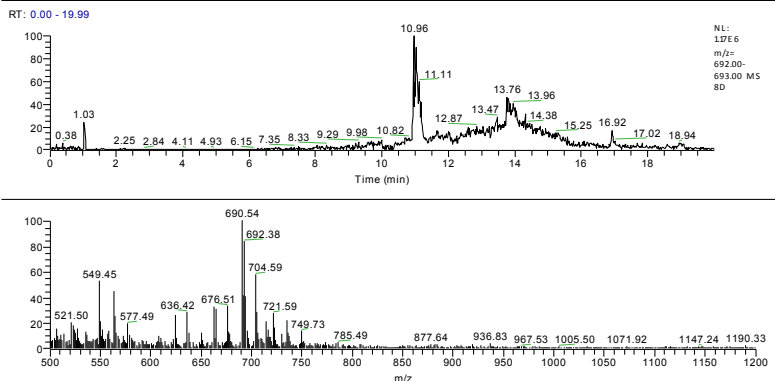
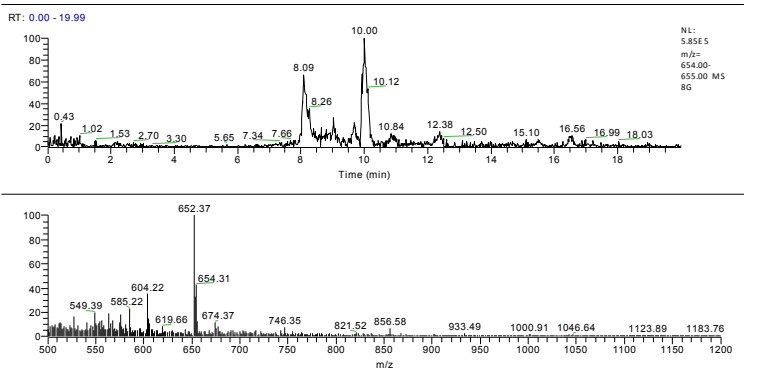
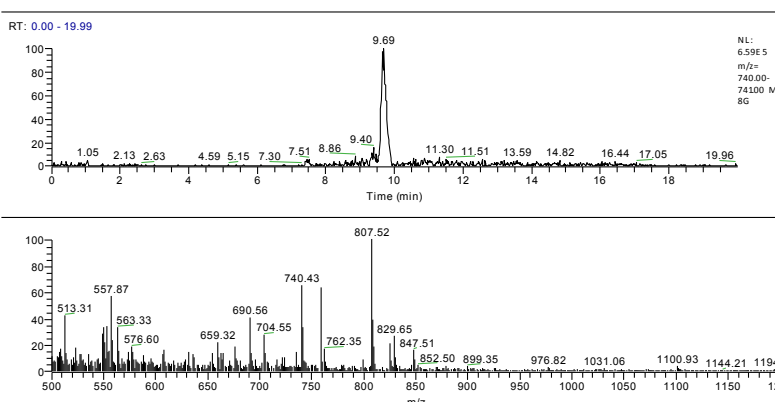
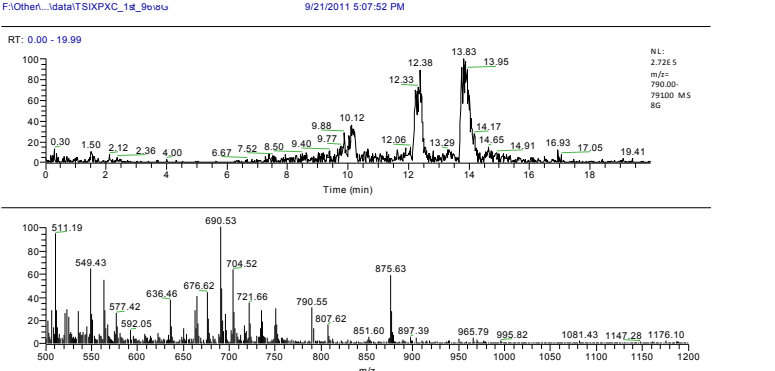


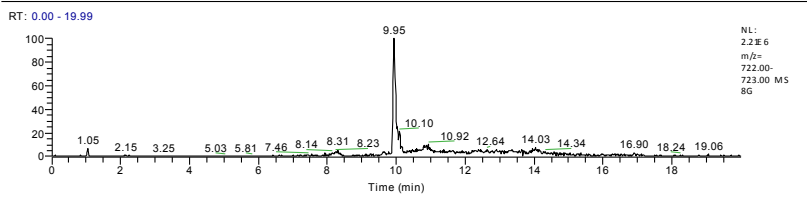
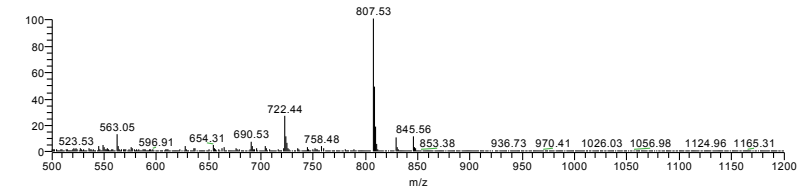
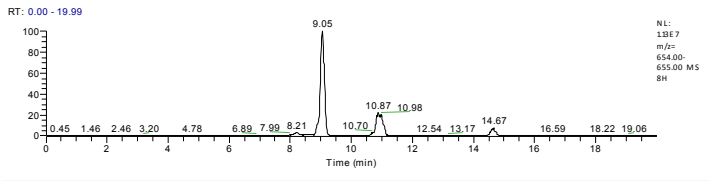
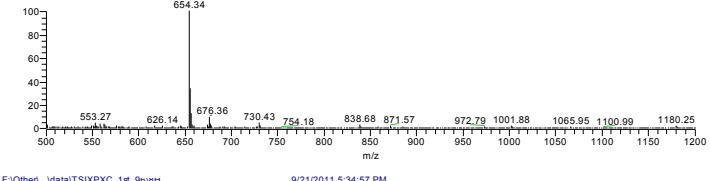
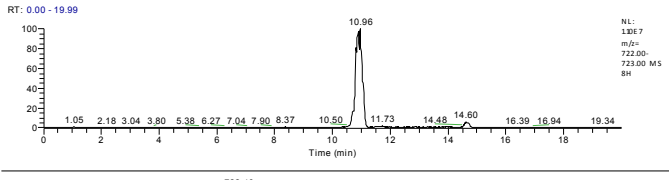
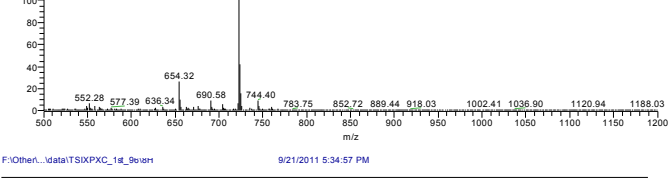
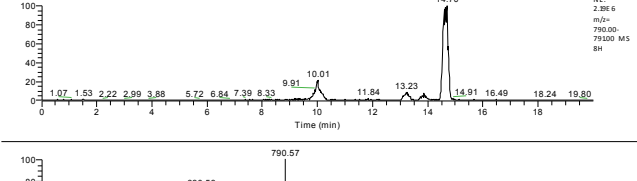
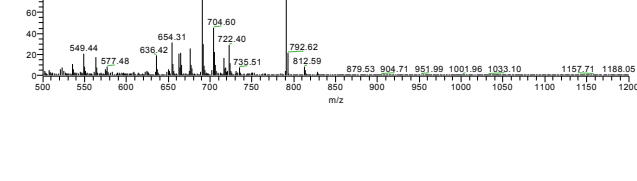
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+2isoprene	820	
dhs+ipr	734	
dhs+2ipr	802	
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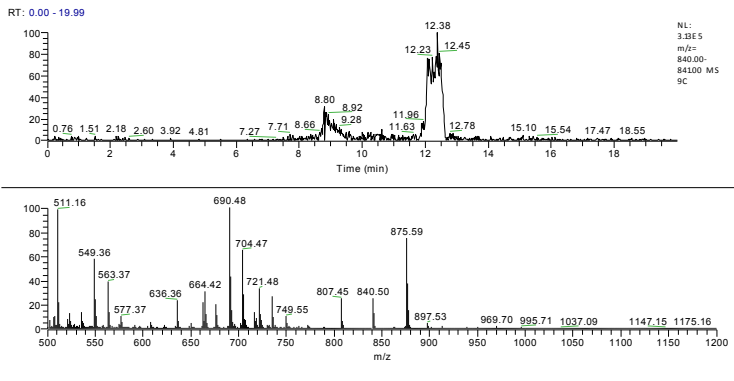
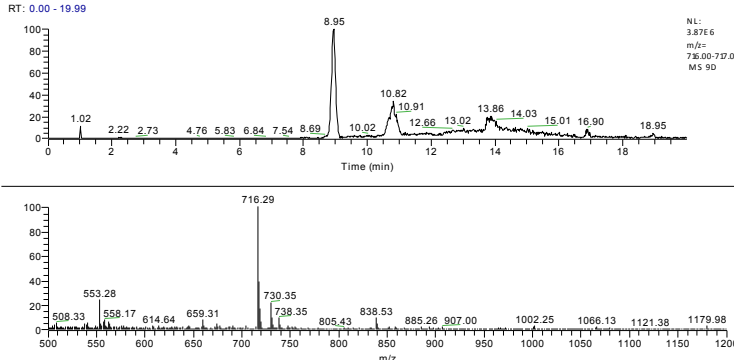
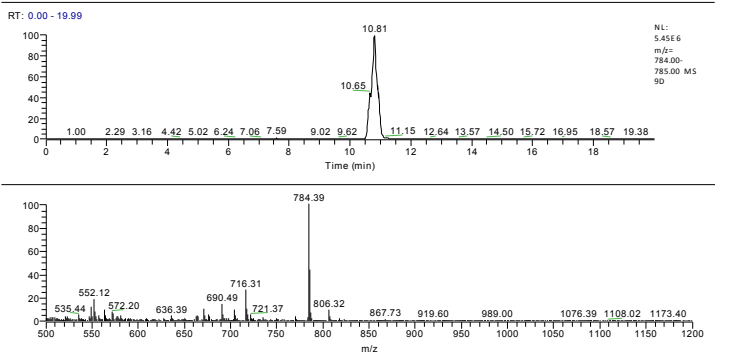
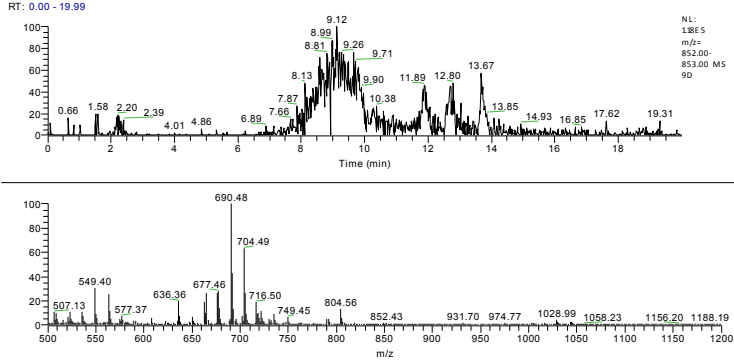
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<p>TSIAPSC</p> <p>+isoprene 710</p> <p>+2isoprene 784</p> <p>dhs+ipr 732</p> <p>dhs+2ipr 804</p>		<p>F:\Other...data\TSIXPXC_1st_9e10u 9/21/2011 3:46:48 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 5.33E5 m/z: 783.00-710.00 MS 8D</p> <p>F:\Other...data\TSIXPXC_1st_9e10u 9/21/2011 3:46:48 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 2.26E5 m/z: 778.00-779.00 MS 8D</p> <p>F:\Other...data\TSIXPXC_1st_9e10u 9/21/2011 3:46:48 PM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 4.32E5 m/z: 760.00-765.00 MS 8D</p>

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<p>TSISPTC (dehydroT) 654 +isoprene 740 dht+ipr 722 dht+2ipr 790</p>		<p>F:\Other...data\TSIXPXC_1st_9618U 9/21/2011 5:07:52 PM</p>  <p>RT: 0.00 - 19.99</p> <p>NL: 5.85E5 m/z= 654.00- 655.00 MS 8G</p> <p>Time (min)</p> <p>m/z</p> <p>F:\Other...data\TSIXPXC_1st_9618G 9/21/2011 5:07:52 PM</p>  <p>RT: 0.00 - 19.99</p> <p>NL: 6.59E5 m/z= 740.00- 741.00 MS 8G</p> <p>Time (min)</p> <p>m/z</p> <p>F:\Other...data\TSIXPXC_1st_9618U 9/21/2011 5:07:52 PM</p>  <p>RT: 0.00 - 19.99</p> <p>NL: 2.72E5 m/z= 790.00- 791.00 MS 8G</p> <p>Time (min)</p> <p>m/z</p>

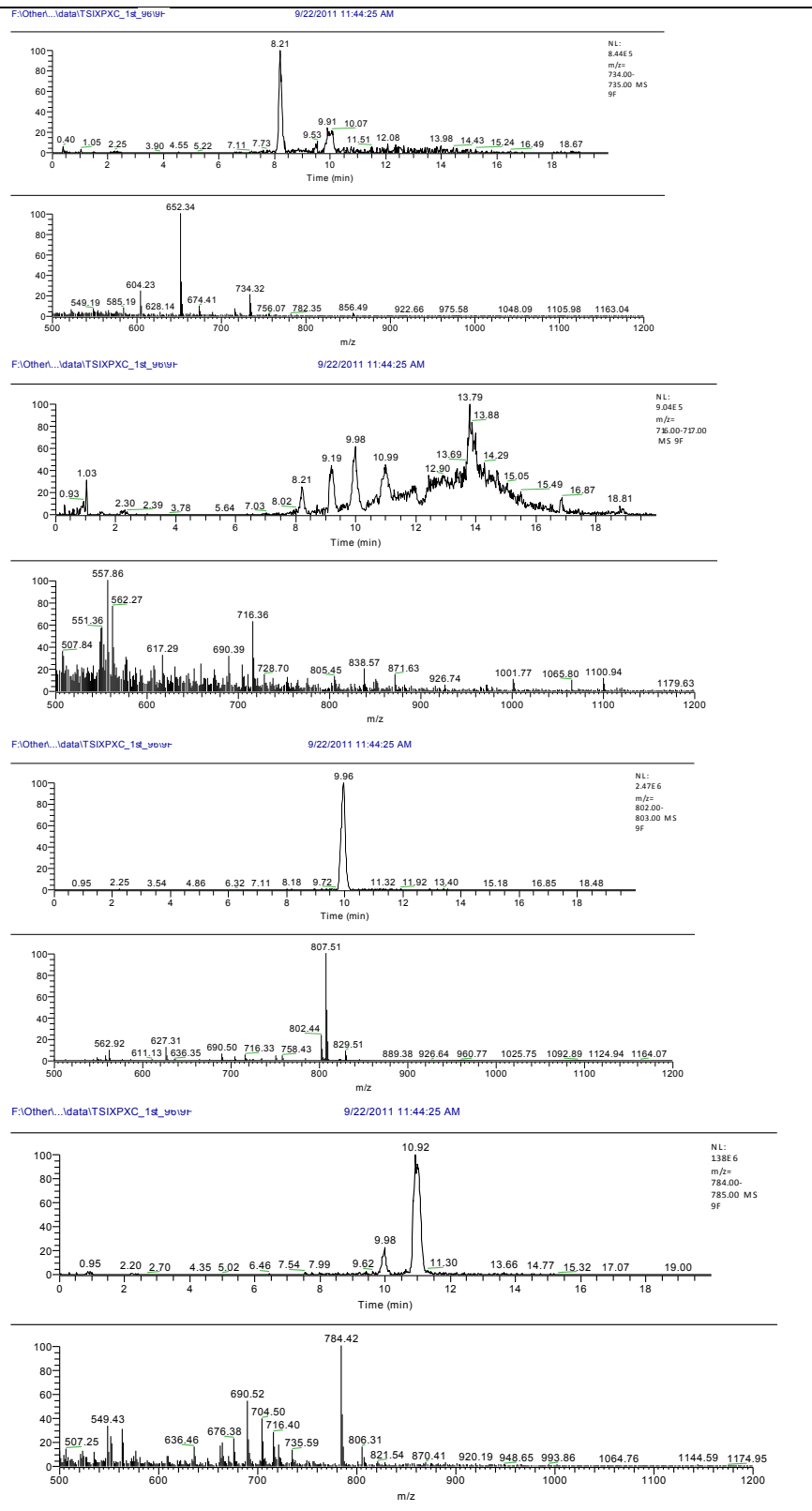
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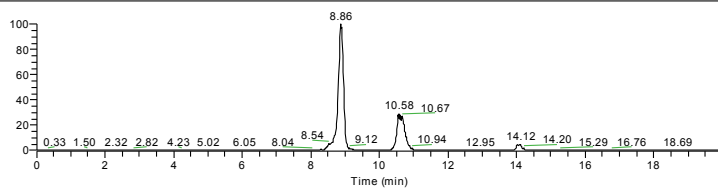
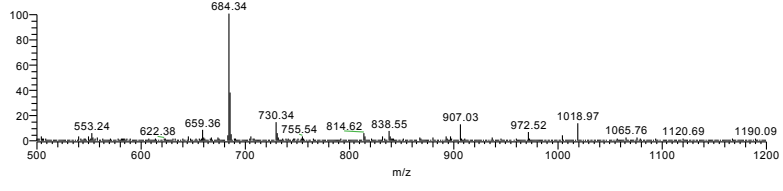
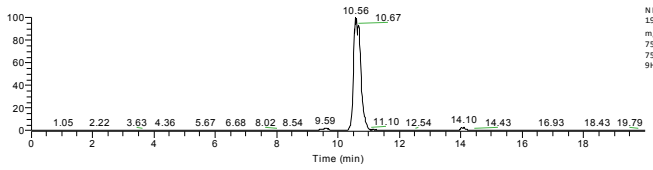
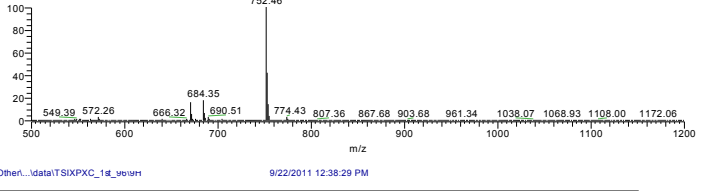
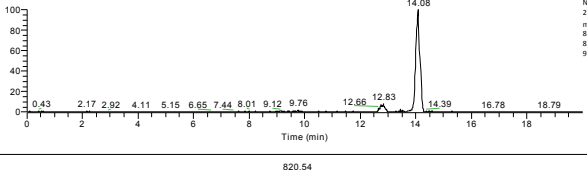
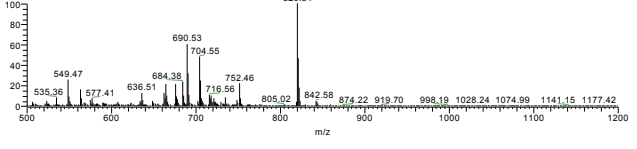
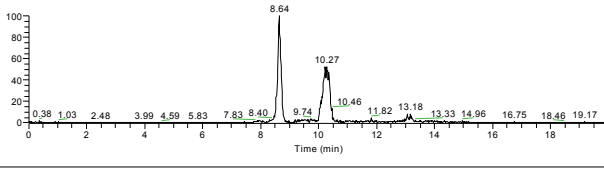
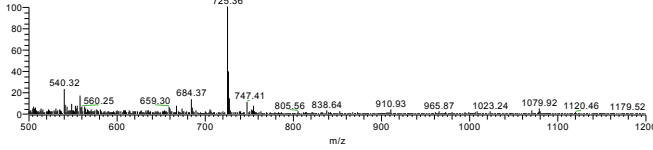
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TSIGPYC	704	F:\Other...data\TSIXPXC_1st_9000A 9/22/2011 9:56:14 AM
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+2isoprene	840	

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<p>TSIGPYC +isoprene +2isoprene</p>	<p>704 772 840</p>	<p>F:\Other...data\TSIXPXC_1st_9e\9c 9/22/2011 10:23:18 AM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p> <p>F:\Other...data\TSIXPXC_1st_9e\9c 9/22/2011 10:23:18 AM</p> <p>RT: 0.00 - 19.99</p> <p>Time (min)</p> <p>m/z</p>

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<p>TSITPMC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>716</p> <p>784</p> <p>852</p>	<p>F:\Other...data\TSIXPXC_1d_9e9u 9/22/2011 10:50:18 AM</p>  <p>RT: 0.00 - 19.99</p> <p>100 80 60 40 20 0</p> <p>1.02 2.22 2.73 4.76 5.83 6.84 7.54 8.69 8.95 10.02 10.82 10.91 12.66 13.02 13.86 14.03 15.01 16.90 18.95</p> <p>Time (min)</p> <p>100 80 60 40 20 0</p> <p>500 550 600 650 700 750 800 850 900 950 1000 1050 1100 1150 1200</p> <p>m/z</p> <p>NL: 3.87E6 m/z= 785.00-77.00 MS 9D</p> <p>F:\Other...data\TSIXPXC_1d_9e9u 9/22/2011 10:50:18 AM</p>  <p>RT: 0.00 - 19.99</p> <p>100 80 60 40 20 0</p> <p>1.00 2.29 3.16 4.42 5.02 6.24 7.06 7.59 9.02 9.62 10.65 10.81 11.15 12.64 13.57 14.50 15.72 16.95 18.57 19.38</p> <p>Time (min)</p> <p>100 80 60 40 20 0</p> <p>500 550 600 650 700 750 800 850 900 950 1000 1050 1100 1150 1200</p> <p>m/z</p> <p>NL: 5.45E6 m/z= 784.00- 785.00 MS 9D</p> <p>F:\Other...data\TSIXPXC_1d_9e9u 9/22/2011 10:50:18 AM</p>  <p>RT: 0.00 - 19.99</p> <p>100 80 60 40 20 0</p> <p>0.66 1.58 2.20 2.39 4.01 4.86 6.89 7.66 7.87 8.13 8.81 8.99 9.12 9.26 9.71 9.90 11.89 12.80 13.67 13.85 14.93 16.85 17.62 19.31</p> <p>Time (min)</p> <p>100 80 60 40 20 0</p> <p>500 550 600 650 700 750 800 850 900 950 1000 1050 1100 1150 1200</p> <p>m/z</p> <p>NL: 1.88E5 m/z= 852.00- 853.00 MS 9D</p>

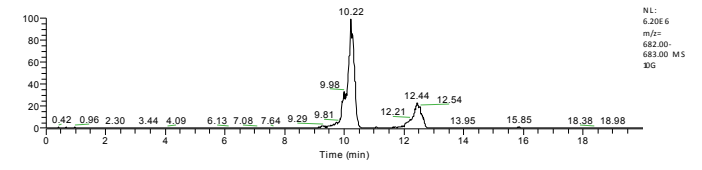
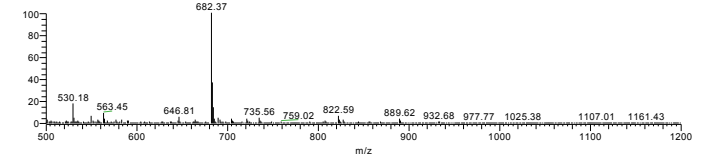
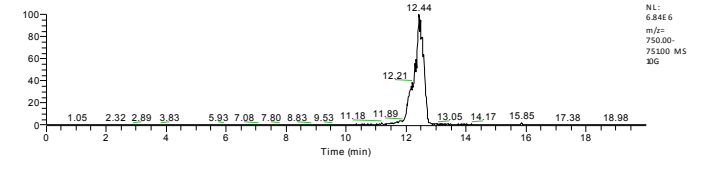
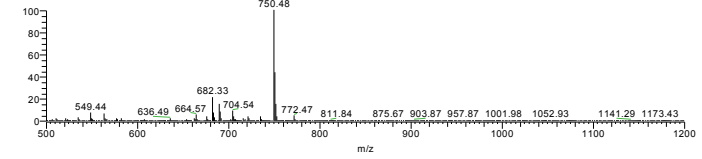
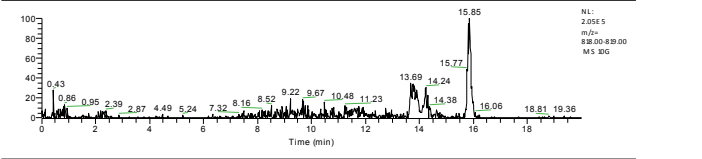
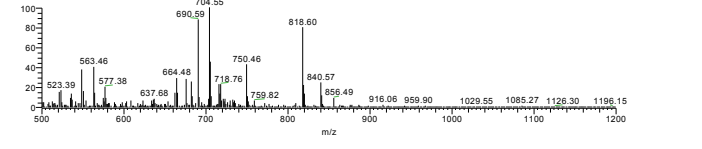
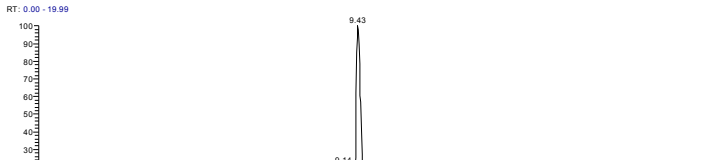
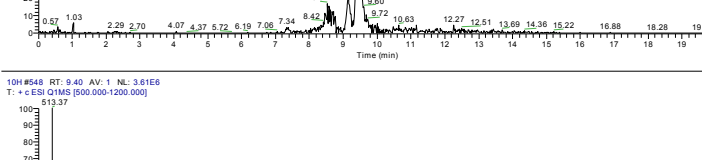
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 (dehydroS) 716
 +isoprene 802
 dhS+ipr 784

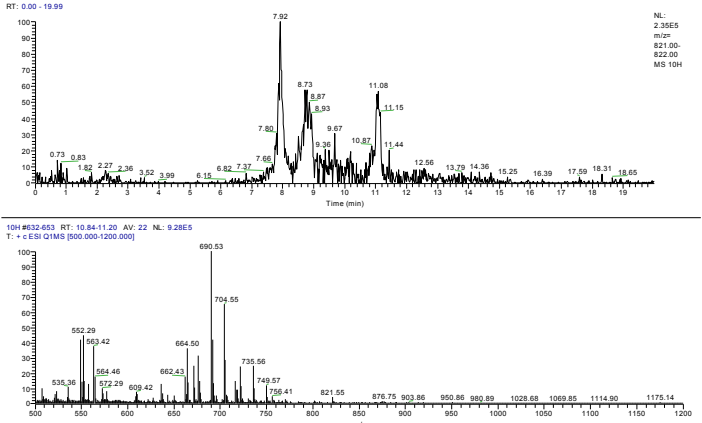
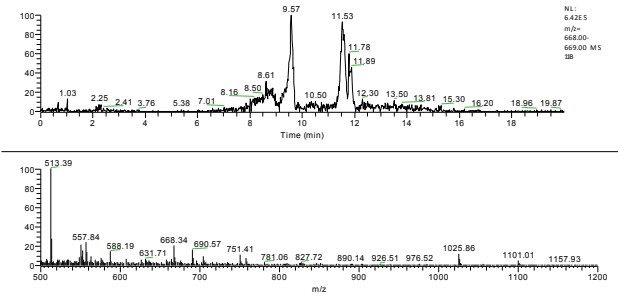
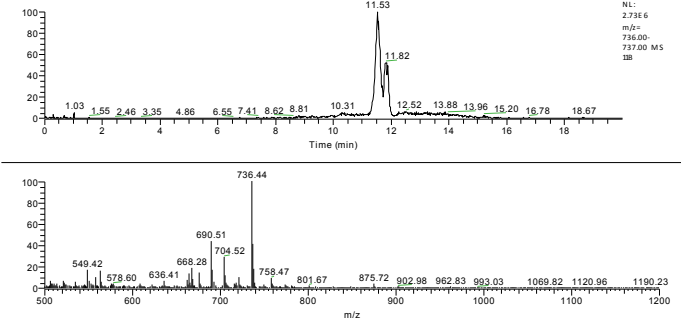
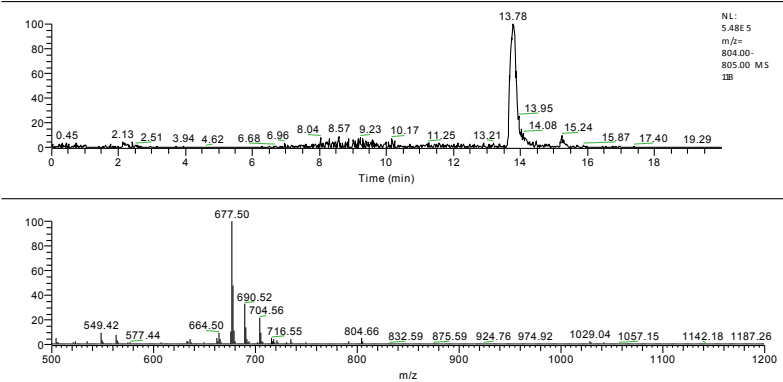


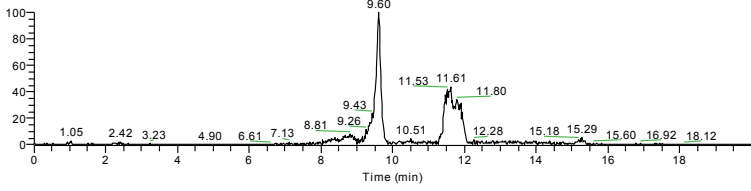
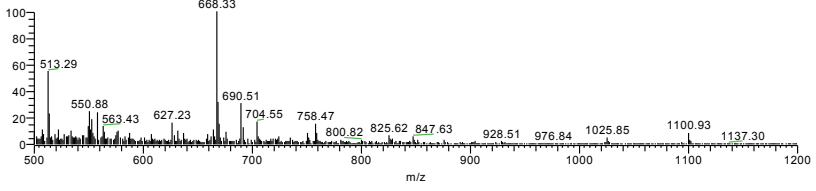
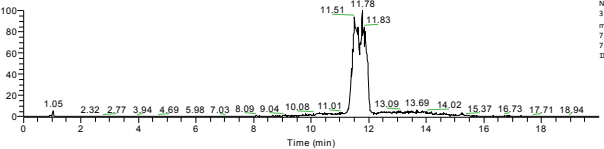
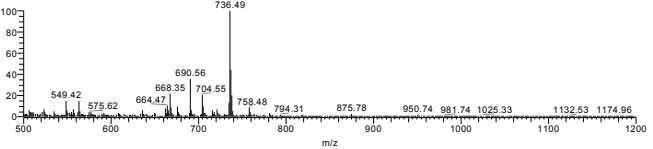
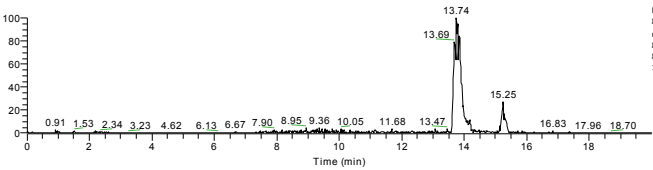
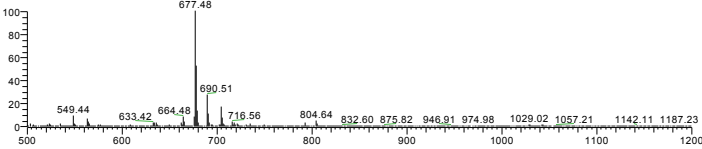
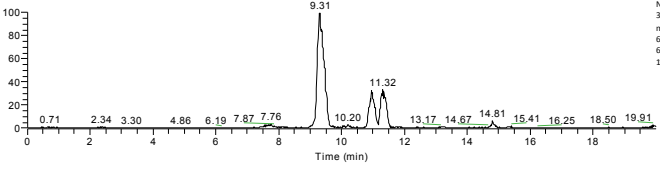
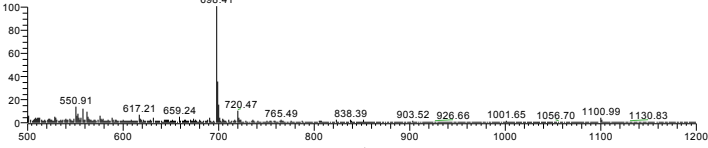
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<p>TSIQPLC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>725</p> <p>793</p> <p>861</p>	<p>F:\Other...data\TSIXPXC_1st_90110A 9/22/2011 1:05:33 PM</p>  <p>NL: 24E6 m/z= 725.00-726.00 MS 9A</p> 

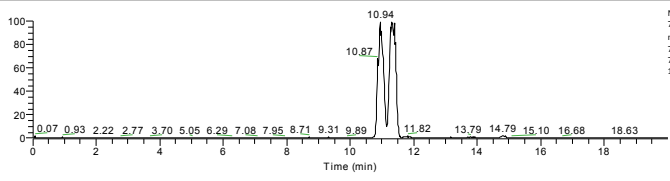
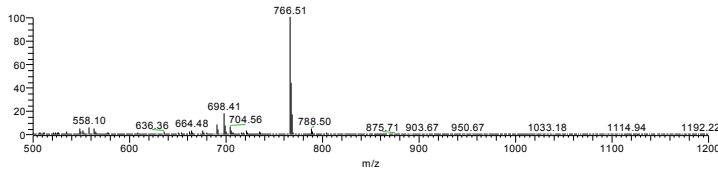
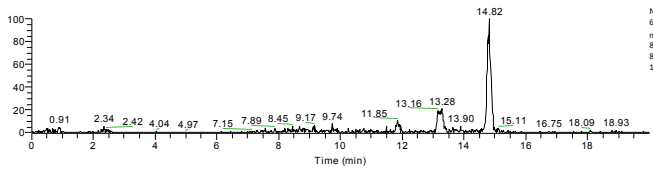
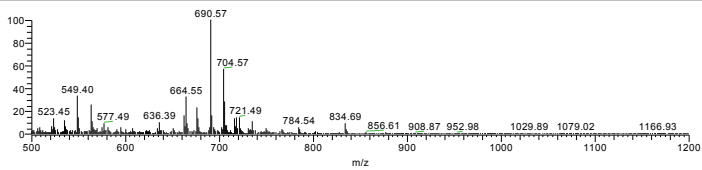
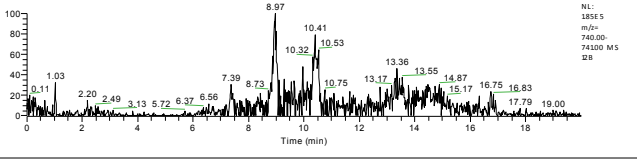
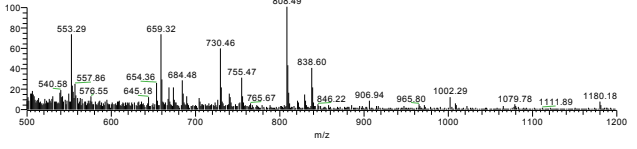
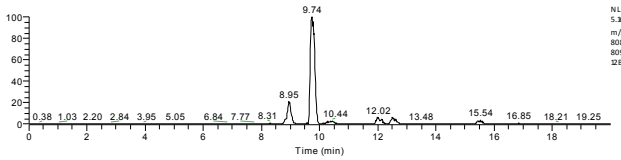
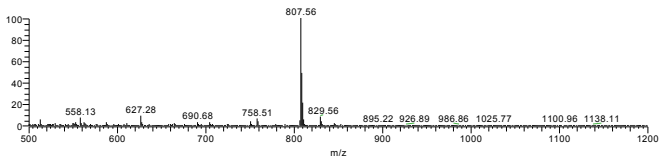
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TSIFPWC +isoprene	885	<p>F:\Other...data\TSIXPXC_1f_96110C 9/22/2011 1:39:36 PM</p> <p>Time (min)</p> <p>NI: 8.40E4 m/z: 885.00- 886.00 MS DC</p> <p>m/z</p>
TSIHPVC +isoprene +2isoprene	720 788 856	<p>F:\Other...data\TSIXPXC_1f_96110C 9/22/2011 2:33:45 PM</p> <p>Time (min)</p> <p>NI: 1.86E6 m/z: 720.00- 722.00 MS DC</p> <p>m/z</p> <p>F:\Other...data\TSIXPXC_1f_96110C 9/22/2011 2:33:45 PM</p> <p>Time (min)</p> <p>NI: 1.86E7 m/z: 788.00- 789.00 MS DC</p> <p>m/z</p>

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+isoprene	786	
+2isoprene	854	
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TSIVPVC	682	<p>F:\Other...data\TSIXPXC_1st_96110G 9/22/2011 3:27:51 PM</p>   <p>F:\Other...data\TSIXPXC_1st_96110G 9/22/2011 3:27:51 PM</p>   <p>F:\Other...data\TSIXPXC_1st_96110G 9/22/2011 3:27:51 PM</p>  
+isoprene	750	
+2isoprene	818	
TSISPNC	754	<p>F:\Other...data\TSIXPXC_1st_96110H 9/22/2011 3:54:54 PM</p>   <p>10H#548 RT: 9.40 AV: 1 NL: 3.61E6 T: + e-ESI Q1MS (500.000-1200.000)</p>
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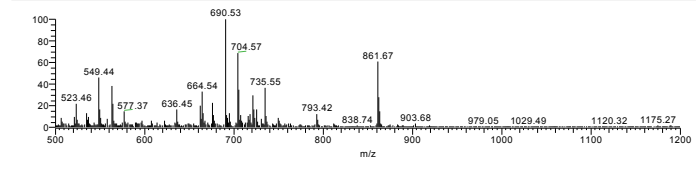
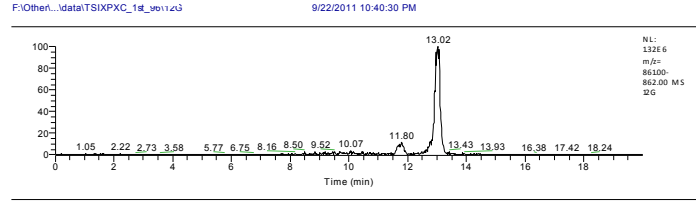
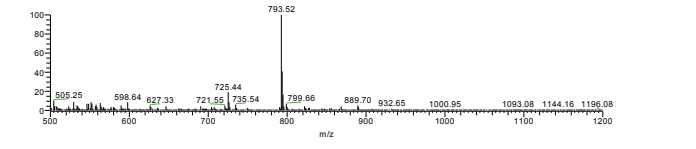
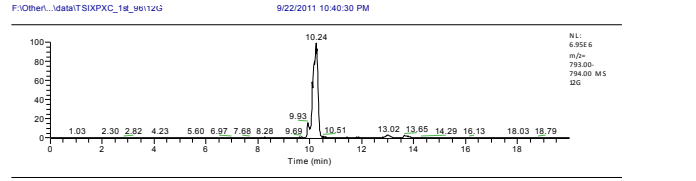
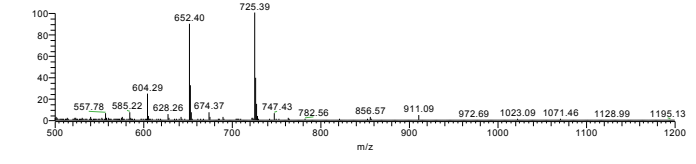
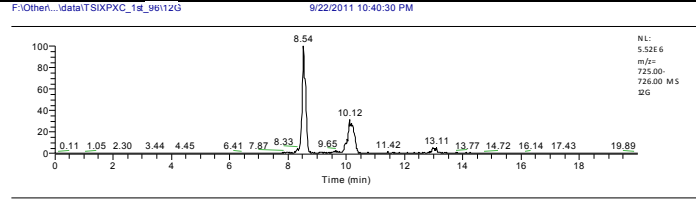
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<p>TSIIPAC +isoprene +2isoprene</p>	<p>668 736 804</p>	<p>F:\Other...data\TSIXPXC_1st_96111B 9/22/2011 4:48:58 PM</p>  <p>F:\Other...data\TSIXPXC_1st_96111B 9/22/2011 4:48:58 PM</p>  <p>F:\Other...data\TSIXPXC_1st_96111B 9/22/2011 4:48:58 PM</p> 

<p>TSIIPAC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>668</p> <p>736</p> <p>804</p>	<p>F:\Other...data\TSIXPXC_18_96111C 9/22/2011 5:16:00 PM</p>  <p>NL: 154E6 m/z= 668.00-669.00 MS IC</p>  <p>F:\Other...data\TSIXPXC_18_96111C 9/22/2011 5:16:00 PM</p>  <p>NL: 3.99E6 m/z= 736.00-737.00 MS IC</p>  <p>F:\Other...data\TSIXPXC_18_96111C 9/22/2011 5:16:00 PM</p>  <p>NL: 8.38E5 m/z= 804.00-805.00 MS IC</p> 
<p>TSITPLC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>698</p> <p>766</p> <p>834</p>	<p>F:\Other...data\TSIXPXC_18_96111D 9/22/2011 5:43:02 PM</p>  <p>NL: 3.93E6 m/z= 698.00-699.00 MS ID</p> 

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<p>TSIQPQC +isoprene +2isoprene</p>	<p>740 808 876</p>	<p>F:\Other...data\TSIXPXC_1st_961128.D 9/22/2011 8:25:17 PM</p>   <p>F:\Other...data\TSIXPXC_1st_961128.D 9/22/2011 8:25:17 PM</p>  

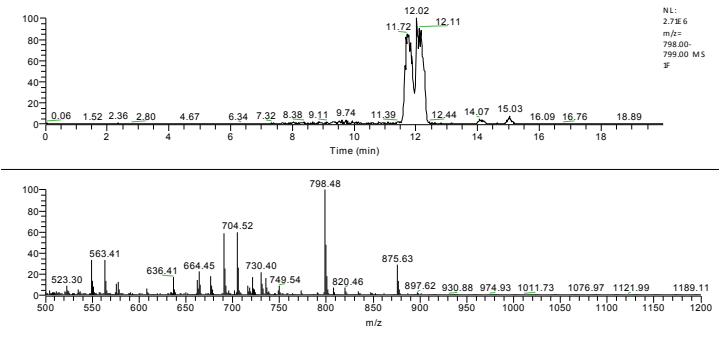
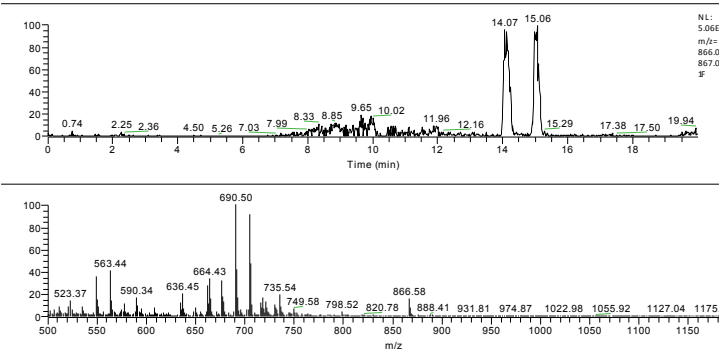
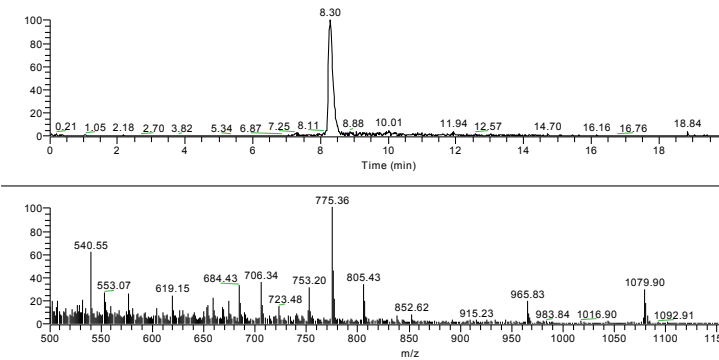
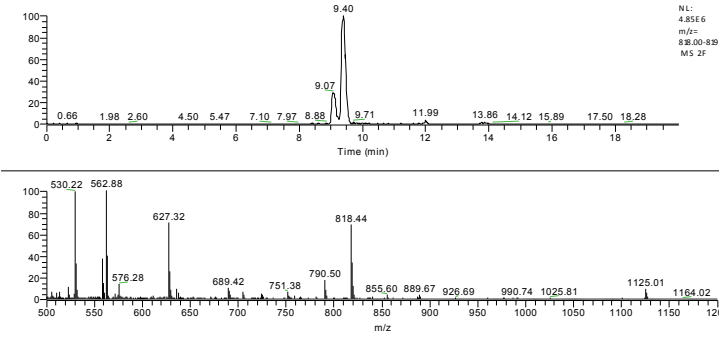
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 +isoprene 793
 +2isoprene 861

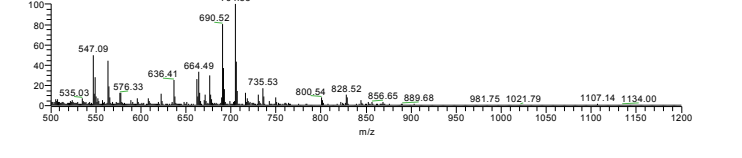
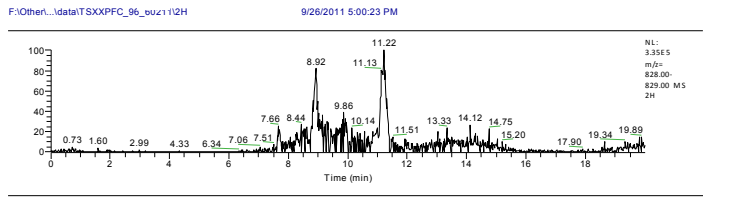
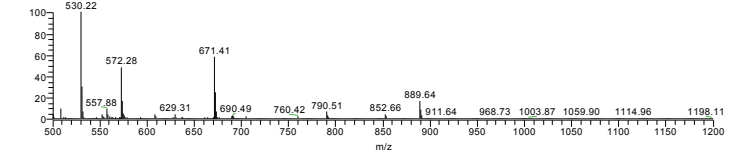
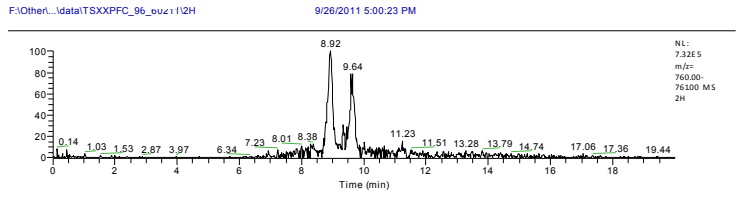
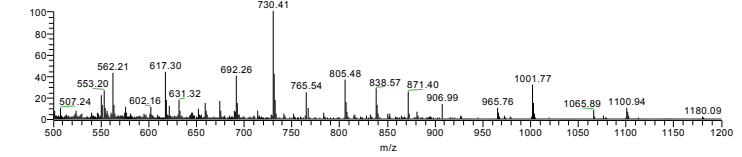
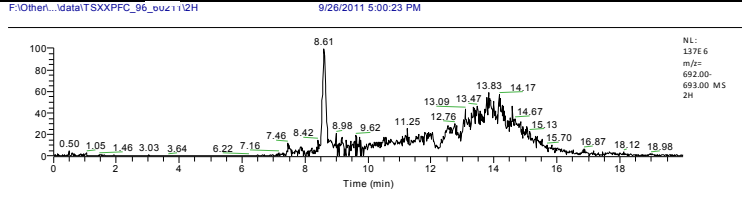


S4C. TSXXPFC

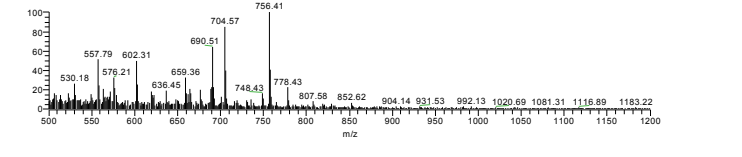
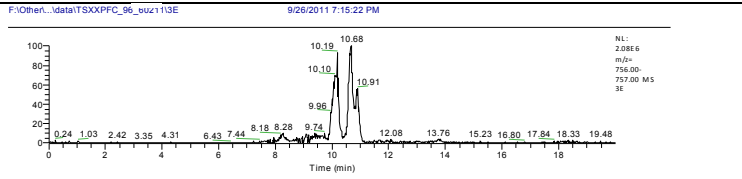
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TSSIPFC	718	<p>F:\Other...data\TSXXPFC_96_b021111E 9/26/2011 12:02:44 PM</p> <p>F:\Other...data\TSXXPFC_96_b021111E 9/26/2011 12:02:44 PM</p>
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+isoprene	798	
+2isoprene	866	

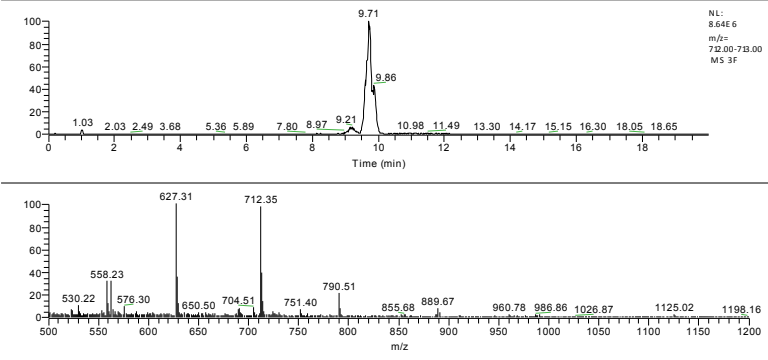
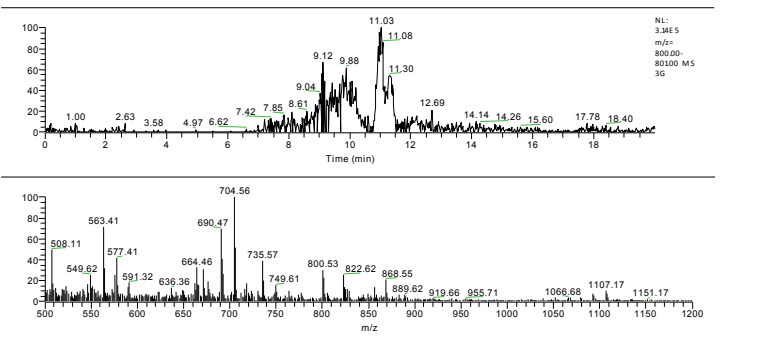
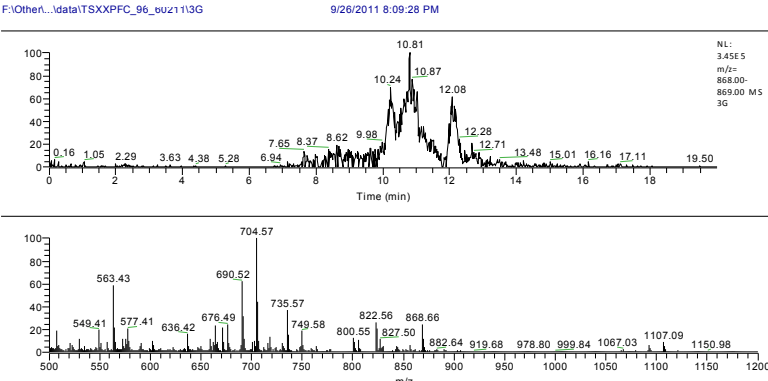
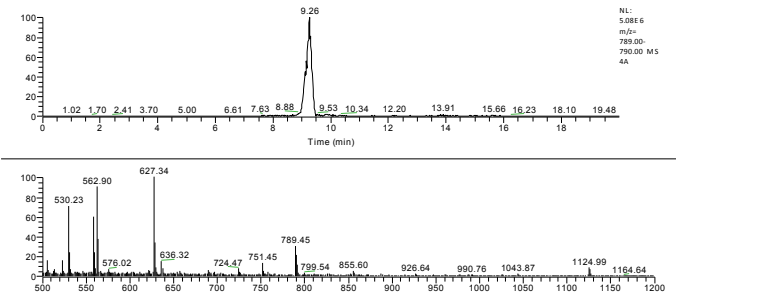
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TSEQPFC	775	<p>F:\Other...data\TSXXPFC_96_buz1112E 9/26/2011 3:38:59 PM</p> 
TSWNPFC	818	<p>F:\Other...data\TSXXPFC_96_buz1112F 9/26/2011 4:06:01 PM</p> 

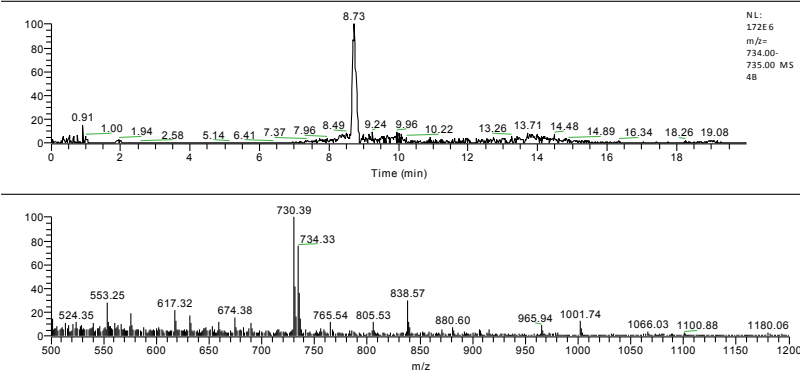
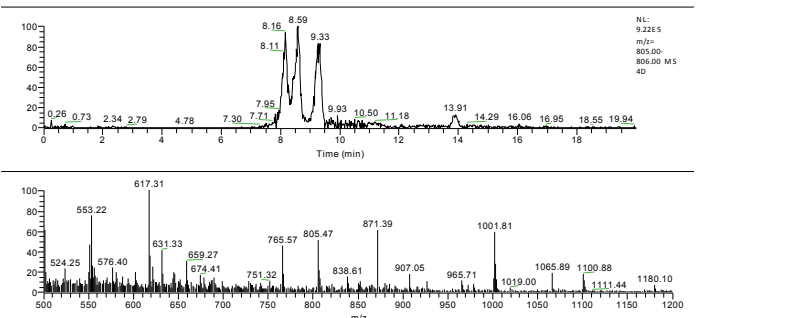
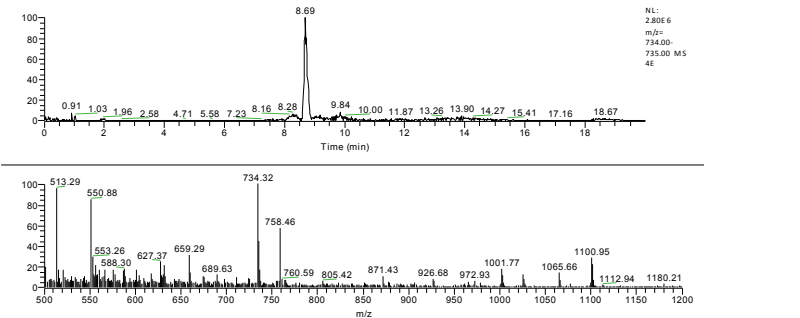
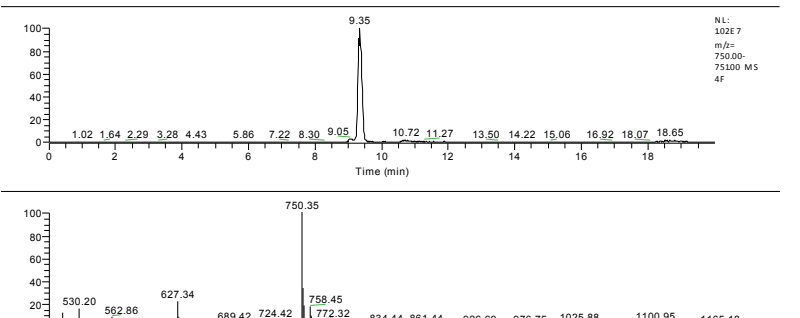
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 +isoprene 760
 +2isoprene 828

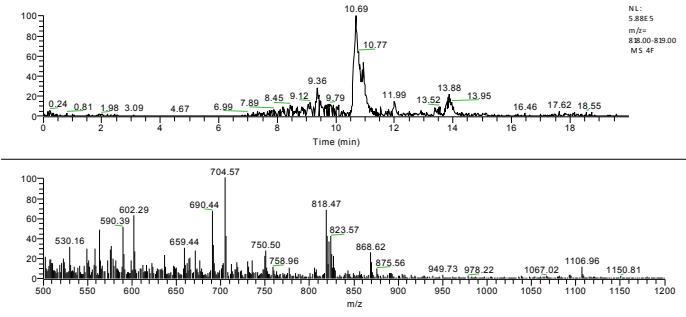
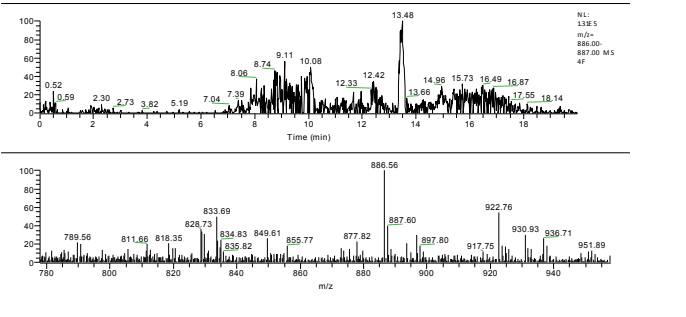
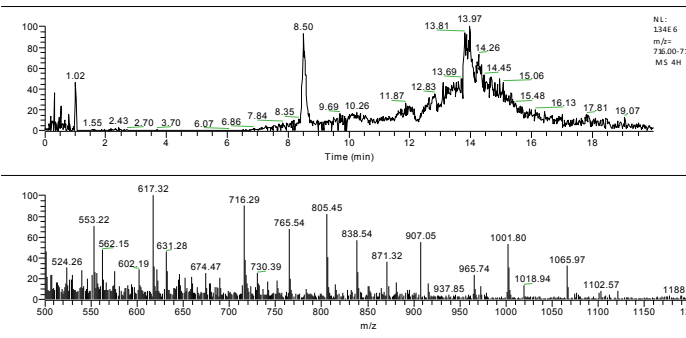
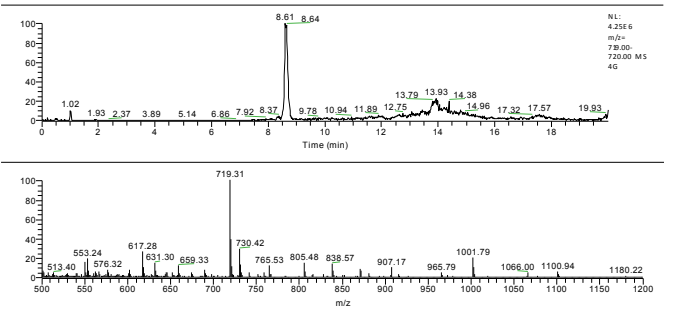


TSAVPFC 688



TSHGPFC	712	<p>F:\Other...data\TSXXPFC_96_euz113F 9/26/2011 7:42:24 PM</p>  <p>Chromatogram (Time vs. Intensity):</p> <ul style="list-style-type: none"> Peak 1: 9.71 min (Intensity ~100) Peak 2: 9.86 min (Intensity ~80) Other labeled peaks: 1.03, 2.03, 2.49, 3.68, 5.36, 5.89, 7.80, 8.97, 9.21, 10.98, 11.49, 13.30, 14.17, 15.15, 16.30, 18.05, 18.65 <p>Mass Spectrum (m/z vs. Intensity):</p> <ul style="list-style-type: none"> Major peaks: 627.31, 712.35 Other labeled peaks: 530.22, 558.23, 576.30, 650.50, 704.51, 751.40, 790.51, 855.68, 889.67, 960.78, 986.86, 1026.87, 1125.02, 1198.16 <p>Metadata: NL: 8.64E 6, m/z: 712.00-718.00, MS 3F</p>
TSVDPFC +isoprene +2isoprene	800 868	<p>F:\Other...data\TSXXPFC_96_euz113G 9/26/2011 8:09:28 PM</p>  <p>Chromatogram (Time vs. Intensity):</p> <ul style="list-style-type: none"> Major peaks: 11.03, 11.08, 11.30 Other labeled peaks: 1.00, 2.63, 3.58, 4.97, 6.62, 7.42, 7.85, 8.81, 9.04, 9.12, 9.88, 12.69, 14.14, 14.26, 15.60, 17.78, 18.40 <p>Mass Spectrum (m/z vs. Intensity):</p> <ul style="list-style-type: none"> Major peaks: 704.56, 690.47 Other labeled peaks: 508.11, 549.62, 563.41, 577.41, 591.32, 636.36, 664.46, 735.57, 749.61, 800.53, 822.62, 868.55, 889.62, 919.66, 955.71, 1066.68, 1107.17, 1151.17 <p>Metadata: NL: 3.44E 5, m/z: 800.00-80100 MS 3G</p> <p>F:\Other...data\TSXXPFC_96_euz113G 9/26/2011 8:09:28 PM</p>  <p>Chromatogram (Time vs. Intensity):</p> <ul style="list-style-type: none"> Major peaks: 10.81, 10.24, 10.87, 12.08 Other labeled peaks: 0.16, 1.05, 2.29, 3.63, 4.38, 5.28, 6.94, 7.65, 8.37, 8.62, 9.98, 12.28, 12.71, 13.48, 15.01, 16.16, 17.11, 19.50 <p>Mass Spectrum (m/z vs. Intensity):</p> <ul style="list-style-type: none"> Major peaks: 704.57, 690.52 Other labeled peaks: 548.41, 563.43, 577.41, 636.42, 676.49, 735.57, 749.58, 800.55, 822.56, 868.66, 882.64, 919.68, 978.80, 999.84, 1067.03, 1107.09, 1150.98 <p>Metadata: NL: 3.45E 5, m/z: 868.00-869.00 MS 3G</p>
TSRDPFC	789	<p>F:\Other...data\TSXXPFC_96_euz114A 9/26/2011 9:03:35 PM</p>  <p>Chromatogram (Time vs. Intensity):</p> <ul style="list-style-type: none"> Major peak: 9.26 min (Intensity ~100) Other labeled peaks: 1.02, 1.70, 2.41, 3.70, 5.00, 6.61, 7.63, 8.88, 9.53, 10.34, 12.20, 13.91, 15.66, 16.23, 18.10, 19.48 <p>Mass Spectrum (m/z vs. Intensity):</p> <ul style="list-style-type: none"> Major peaks: 627.34, 789.45 Other labeled peaks: 530.23, 562.90, 575.02, 636.32, 724.47, 751.45, 799.54, 855.60, 926.64, 990.76, 1043.87, 1124.99, 1164.64 <p>Metadata: NL: 5.08E 6, m/z: 789.00-790.00 MS 4A</p>

TSESPFC	734	<p>F:\Other...data\TSXXPFC_96_buz114B 9/26/2011 9:30:37 PM</p>  <p>Chromatogram peaks (min): 0.91, 1.00, 1.94, 2.58, 5.14, 6.41, 7.37, 7.96, 8.49, 8.73, 9.24, 9.96, 10.22, 13.26, 13.71, 14.48, 14.89, 16.34, 18.26, 19.08</p> <p>Mass spectrum peaks (m/z): 524.35, 553.25, 617.32, 674.38, 730.39, 734.33, 765.54, 805.53, 838.57, 880.60, 965.94, 1001.74, 1066.03, 1100.88, 1180.06</p> <p>Metadata: NL: 172E6, m/z: 734.00, 735.00 MS, 4B</p>
TSMRPFC	805	<p>F:\Other...data\TSXXPFC_96_802114D 9/26/2011 10:24:41 PM</p>  <p>Chromatogram peaks (min): 0.26, 0.73, 2.34, 2.79, 4.78, 7.30, 7.71, 7.95, 8.16, 8.59, 9.33, 9.93, 10.50, 11.18, 13.91, 14.29, 16.06, 16.95, 18.55, 19.94</p> <p>Mass spectrum peaks (m/z): 524.25, 553.22, 576.40, 617.31, 631.33, 659.27, 674.41, 751.32, 765.57, 805.47, 838.61, 871.39, 907.05, 965.71, 1019.00, 1065.89, 1100.88, 1111.44, 1180.10</p> <p>Metadata: NL: 9.22E5, m/z: 805.00, 806.00 MS, 4D</p>
TSESPFC	734	<p>F:\Other...data\TSXXPFC_96_buz114E 9/26/2011 10:51:43 PM</p>  <p>Chromatogram peaks (min): 0.91, 1.03, 1.96, 2.58, 4.71, 5.58, 7.23, 8.16, 8.28, 8.69, 9.84, 10.00, 11.87, 13.26, 13.90, 14.27, 15.41, 17.16, 18.67</p> <p>Mass spectrum peaks (m/z): 513.29, 550.88, 553.26, 558.30, 627.37, 659.29, 689.63, 734.32, 758.46, 760.59, 805.42, 871.43, 926.68, 972.93, 1001.77, 1065.66, 1100.95, 1112.94, 1180.21</p> <p>Metadata: NL: 2.80E6, m/z: 734.00, 735.00 MS, 4E</p>
TSMTPFC	750	<p>F:\Other...data\TSXXPFC_96_buz114F 9/26/2011 11:18:47 PM</p>  <p>Chromatogram peaks (min): 1.02, 1.64, 2.29, 3.28, 4.43, 5.86, 7.22, 8.30, 9.05, 9.35, 10.72, 11.27, 13.50, 14.22, 15.06, 16.92, 18.07, 18.65</p> <p>Mass spectrum peaks (m/z): 530.20, 562.86, 627.34, 689.42, 724.42, 750.35, 758.45, 772.32, 834.44, 861.44, 926.69, 976.75, 1025.88, 1100.95, 1165.18</p> <p>Metadata: NL: 102E7, m/z: 750.00, 75100 MS, 4F</p>

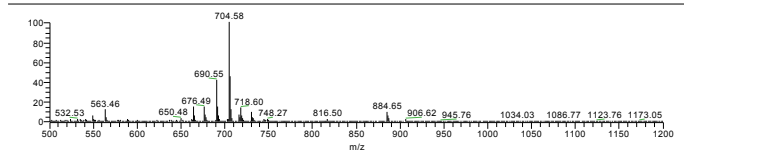
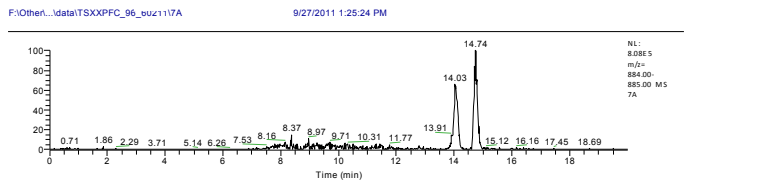
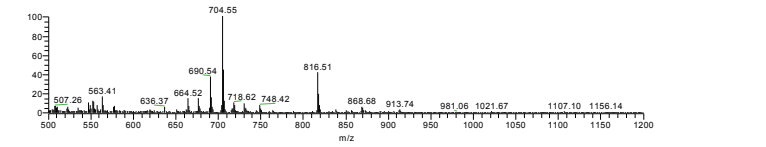
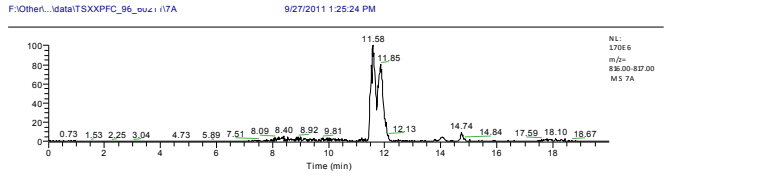
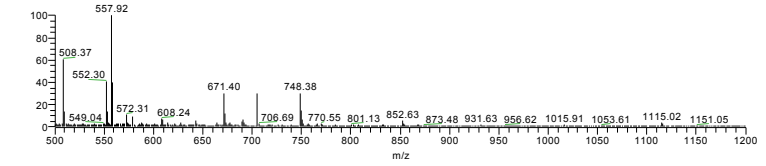
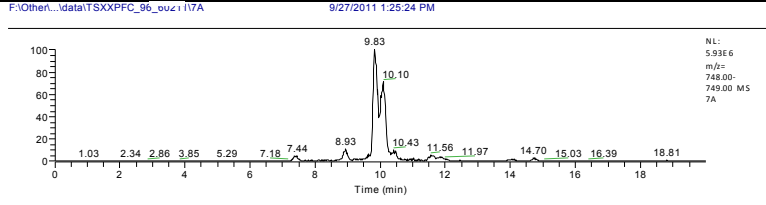
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TSNSPFC	719	<p>F:\Other...data\TSXXPFC_96_buz114G 9/26/2011 11:45:49 PM</p> 

TSTTPFC	716	<p>F:\Other...data\TSXXPFC_96_buz1114H 9/27/2011 12:12:52 AM</p> <p>Chromatogram peaks (min): 1.02, 1.55, 2.43, 2.70, 3.70, 6.07, 6.86, 7.84, 8.35, 8.50, 9.69, 10.26, 11.87, 12.83, 13.69, 13.81, 13.97, 14.26, 14.45, 15.06, 15.48, 16.13, 17.81, 19.07</p> <p>Mass spectrum peaks (m/z): 524.26, 553.22, 562.15, 602.19, 631.28, 674.47, 716.29, 730.39, 765.54, 805.45, 838.54, 871.32, 907.05, 937.85, 965.74, 1001.80, 1018.94, 1065.97, 1102.57, 1188.82</p> <p>Metadata: NL: 134E6, m/z: 786.00-717.00, MS 4H</p>
TSLMPFC	762	<p>F:\Other...data\TSXXPFC_96_buz1115A 9/27/2011 12:39:54 AM</p> <p>Chromatogram peaks (min): 0.35, 1.93, 2.99, 3.85, 4.74, 6.46, 7.49, 7.87, 9.79, 10.10, 11.85, 12.06, 14.22, 14.72, 15.44, 18.03, 19.73</p> <p>Mass spectrum peaks (m/z): 528.62, 552.30, 557.93, 572.29, 608.35, 671.40, 704.60, 756.68, 762.37, 784.38, 852.63, 889.31, 938.59, 1015.82, 1053.92, 1115.03, 1154.03</p> <p>Metadata: NL: 5.37E6, m/z: 762.00, 763.00 MS, SA</p>
TSVRPFC	773	<p>F:\Other...data\TSXXPFC_96_buz1115E 9/27/2011 2:28:02 AM</p> <p>Chromatogram peaks (min): 0.08, 1.00, 1.50, 2.67, 3.85, 4.78, 6.72, 7.54, 8.08, 8.73, 9.31, 9.43, 9.50, 9.59, 10.02, 11.87, 12.13, 13.18, 14.98, 17.13, 17.97, 19.29, 19.89</p> <p>Mass spectrum peaks (m/z): 530.21, 572.25, 627.31, 671.38, 689.42, 733.49, 751.23, 773.49, 790.48, 838.42, 889.65, 902.85, 967.76, 988.73, 1081.00, 1125.10, 1198.19</p> <p>Metadata: NL: 1.85E6, m/z: 773.00, 774.00 MS, SE</p>
TSWSPFC	791	<p>F:\Other...data\TSXXPFC_96_buz1115G 9/27/2011 3:22:08 AM</p> <p>Chromatogram peaks (min): 0.31, 0.93, 1.93, 3.32, 4.30, 5.65, 7.58, 8.33, 9.25, 9.67, 10.22, 12.02, 13.95, 14.48, 16.95, 19.03, 19.51</p> <p>Mass spectrum peaks (m/z): 530.20, 558.23, 621.99, 627.31, 636.32, 689.46, 781.43, 791.41, 813.39, 838.57, 889.67, 911.67, 967.76, 988.80, 1101.93, 1139.08, 1198.27</p> <p>Metadata: NL: 9.73E6, m/z: 792.00 MS, SG</p>

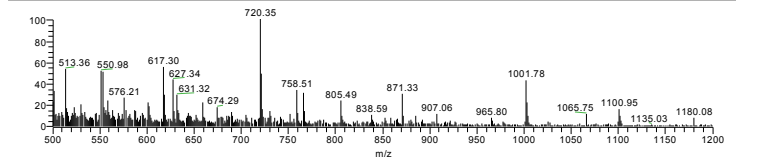
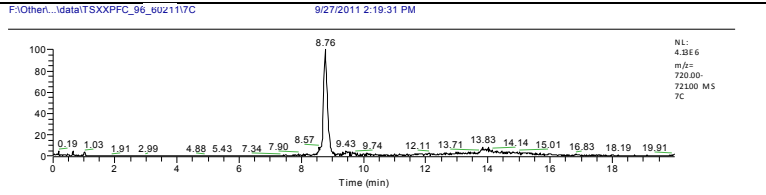
TSVMPFC 748

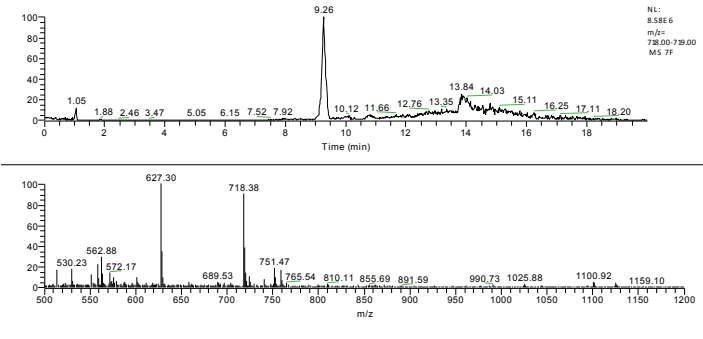
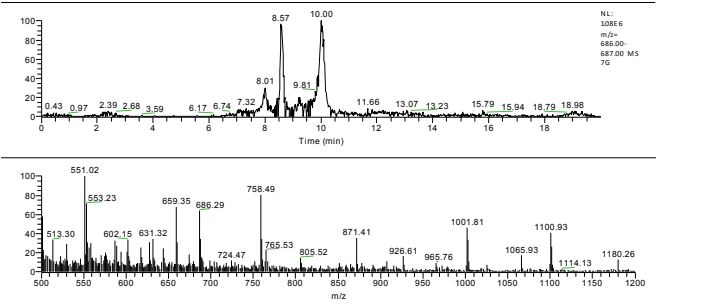
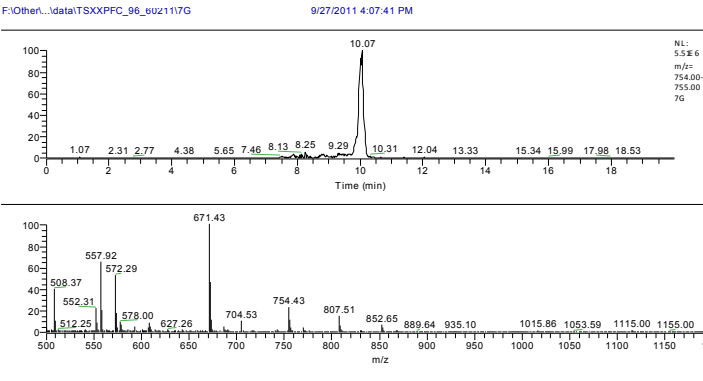
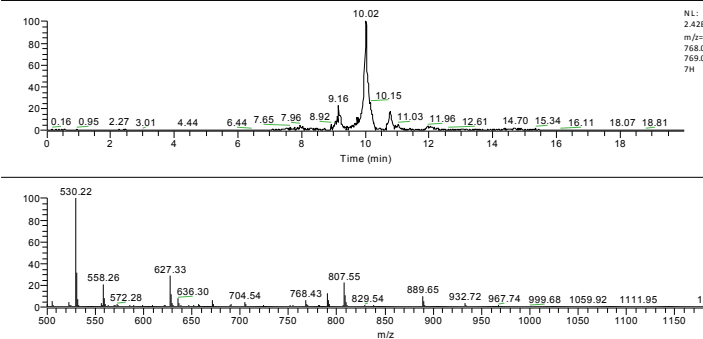
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+2isoprene 884



TSTTPFC 720

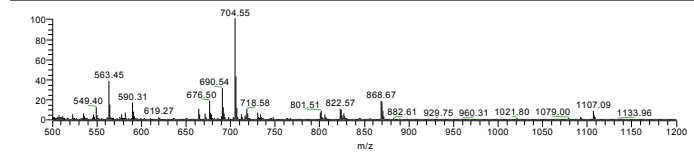
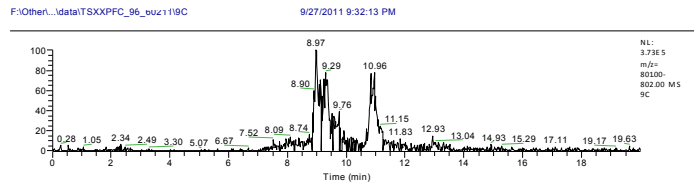
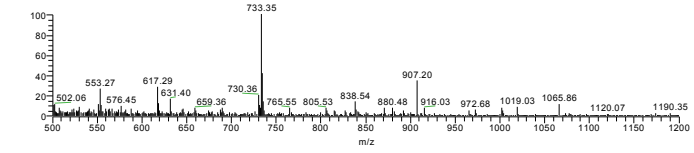
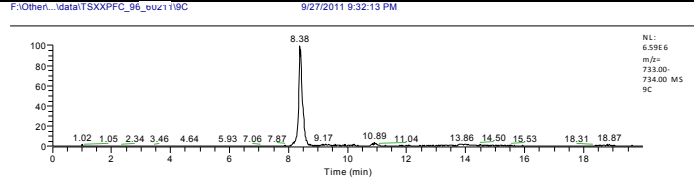


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<p>TSAPPFC +isoprene</p>	<p>686 754</p>	<p>F:\Other...data\TSXXPFC_96_buz117G 9/27/2011 4:07:41 PM</p>  <p>Chromatogram peaks (min): 0.43, 0.97, 2.39, 2.68, 3.59, 6.17, 6.74, 7.32, 8.57, 9.81, 10.00, 11.66, 13.07, 13.23, 15.79, 15.94, 18.79, 18.98</p> <p>Mass spectrum peaks (m/z): 513.30, 551.02, 553.23, 602.15, 631.32, 659.35, 686.29, 724.47, 758.49, 785.53, 871.41, 926.61, 965.76, 1001.81, 1065.93, 1100.93, 1114.13, 1180.26</p> <p>Parameters: NL: 1.08E6, m/z: 686.00-687.00, MS 7G</p> <p>F:\Other...data\TSXXPFC_96_buz117G 9/27/2011 4:07:41 PM</p>  <p>Chromatogram peaks (min): 1.07, 2.31, 2.77, 4.38, 5.65, 7.46, 8.13, 8.25, 9.29, 10.07, 10.31, 12.04, 13.33, 15.34, 15.99, 17.98, 18.53</p> <p>Mass spectrum peaks (m/z): 508.37, 552.31, 557.92, 572.29, 578.00, 627.26, 671.43, 704.53, 754.43, 807.51, 852.65, 889.64, 935.10, 1015.86, 1053.59, 1115.00, 1155.00</p> <p>Parameters: NL: 5.53E6, m/z: 754.00-755.00, MS 7G</p>
<p>TSIHPFC +isoprene +2isoprene</p>	<p>768 836 904</p>	<p>F:\Other...data\TSXXPFC_96_buz117H 9/27/2011 4:34:43 PM</p>  <p>Chromatogram peaks (min): 0.16, 0.95, 2.27, 3.01, 4.44, 6.44, 7.65, 7.96, 8.92, 9.16, 10.02, 10.15, 11.03, 11.96, 12.61, 14.70, 15.34, 16.11, 18.07, 18.81</p> <p>Mass spectrum peaks (m/z): 530.22, 558.26, 627.33, 636.30, 704.54, 768.43, 807.55, 829.54, 889.65, 932.72, 967.74, 999.68, 1059.92, 1111.95, 1198.10</p> <p>Parameters: NL: 2.42E6, m/z: 768.00-769.00, MS 7H</p>

		<p>F:\Other...data\TSXXPFC_06_buz117H 9/27/2011 4:34:43 PM</p> <p>NL: 10716 m/z: 836.00 837.00 MS 7H</p> <p>F:\Other...data\TSXXPFC_06_buz117H 9/27/2011 4:34:43 PM</p> <p>NL: 5375 m/z: 954.00 955.00 MS 7H</p>
TSRSPFC	761	<p>F:\Other...data\TSXXPFC_06_buz118A 9/27/2011 5:01:46 PM</p> <p>NL: 672E5 m/z: 762.00 762.00 MS 8A</p>
TSDQPC	761	<p>F:\Other...data\TSXXPFC_06_buz118E 9/27/2011 6:49:58 PM</p> <p>NL: 357E6 m/z: 761.00 762.00 MS 8E</p>

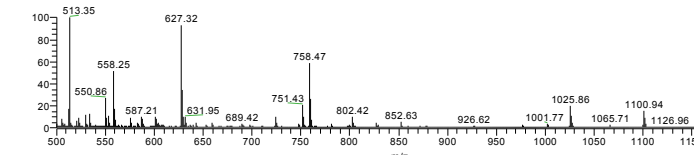
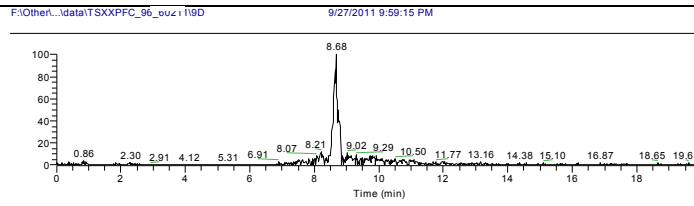
TSTNPFC
+isoprene

733
801



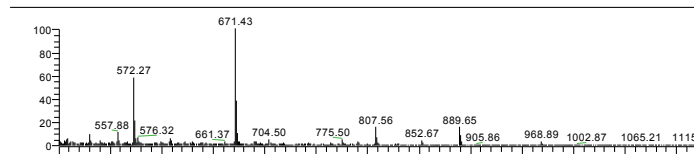
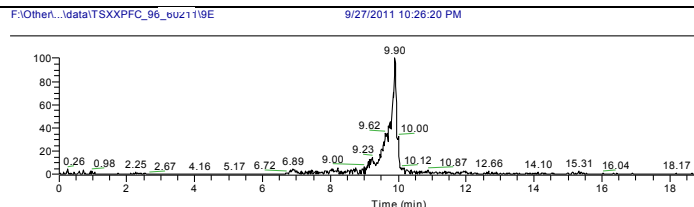
TSRQFC

802

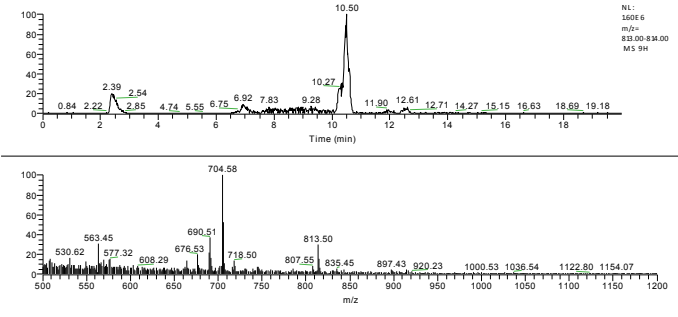
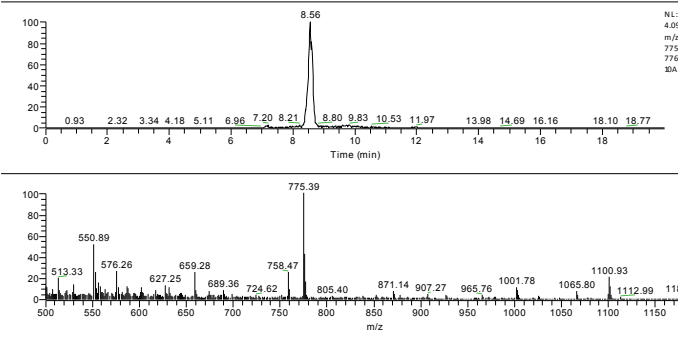
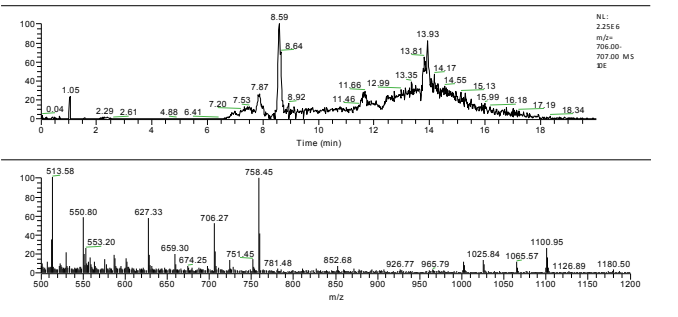
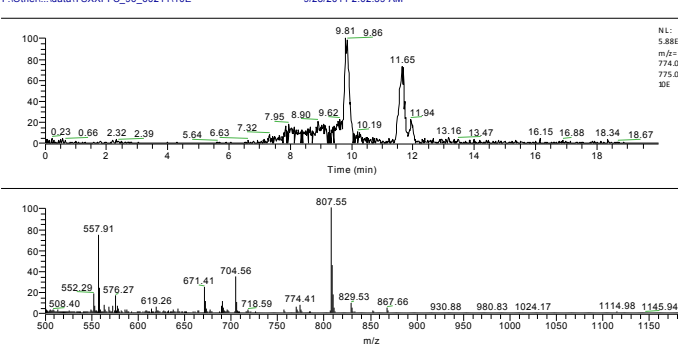


TSRTPFC

775

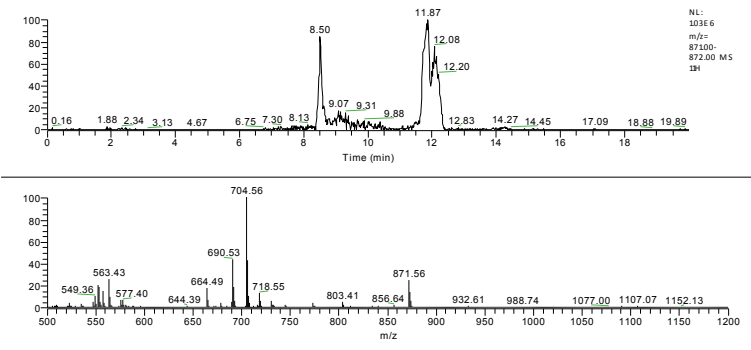
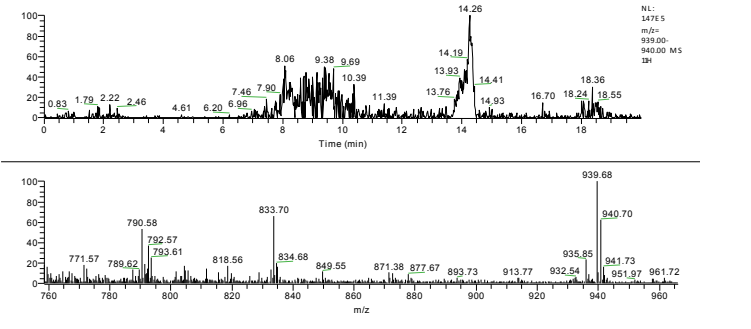
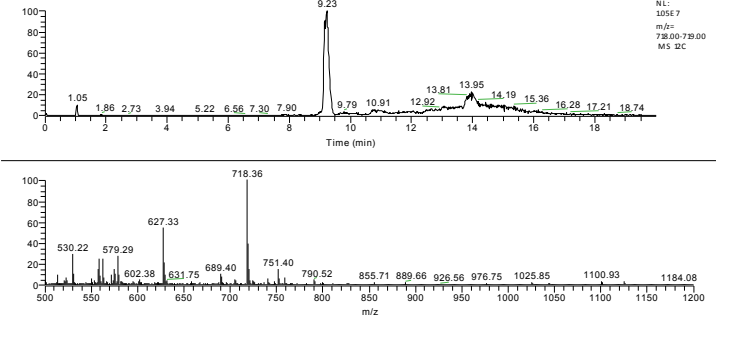
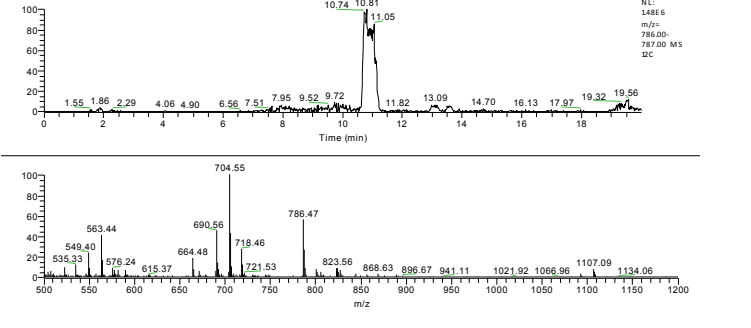


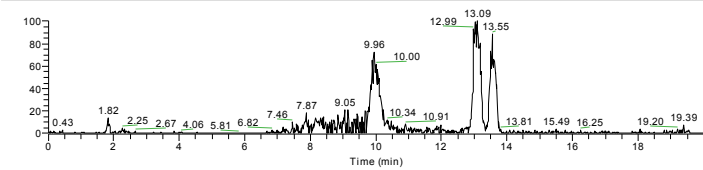
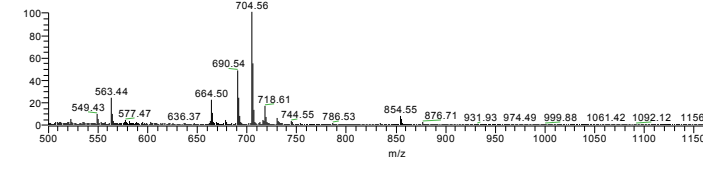
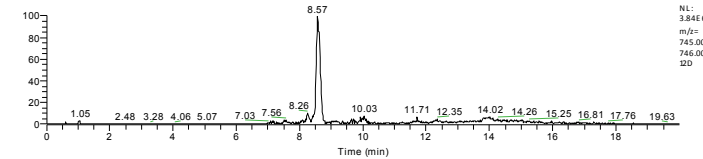
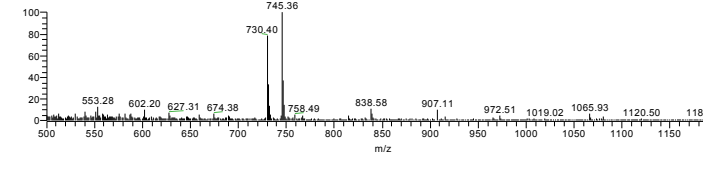
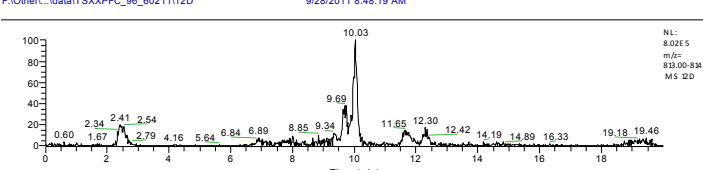
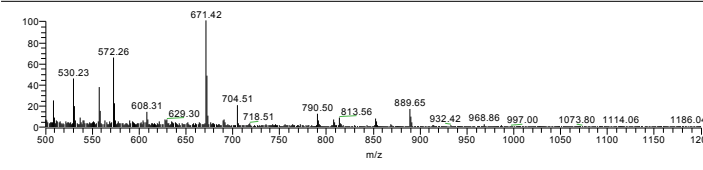
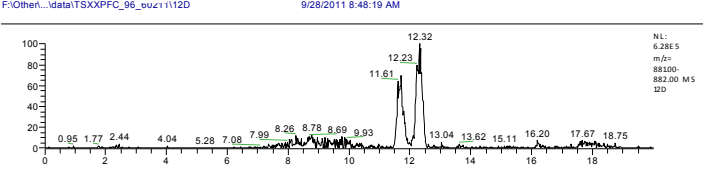
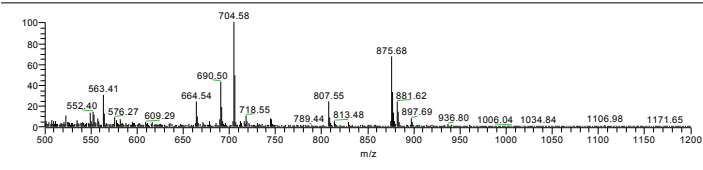
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TSVPPFC +isoprene	714 782	<p>F:\Other...data\TSXXPFC_96_u02119G 9/27/2011 11:20:24 PM</p> <p>NL: 6.88E6 m/z: 782.00-783.00 MS 9G</p> <p>F:\Other...data\TSXXPFC_96_u02119G 9/27/2011 11:20:24 PM</p> <p>NL: 2.44E6 m/z: 782.00-783.00 MS 9G</p>
TSLNPFC +isoprene	745 813	<p>F:\Other...data\TSXXPFC_96_u02119H 9/27/2011 11:47:26 PM</p> <p>NL: 3.85E6 m/z: 745.00-746.00 MS 9H</p>

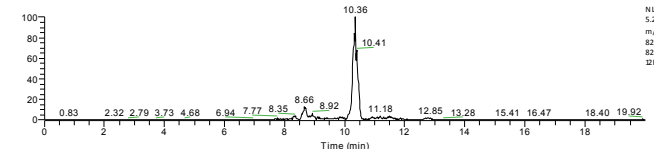
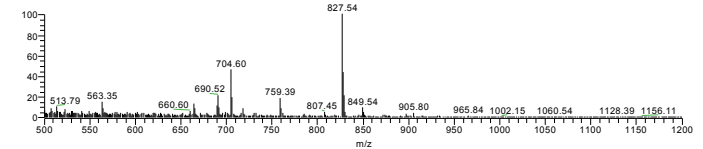
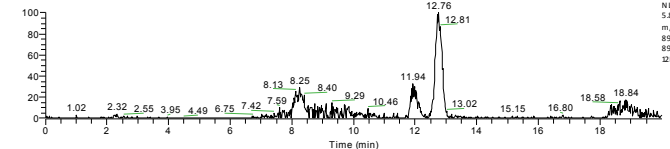
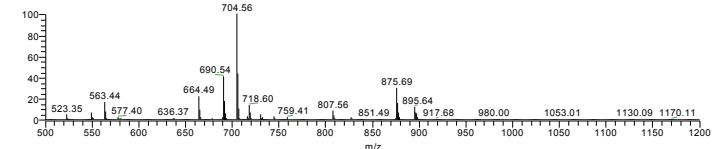
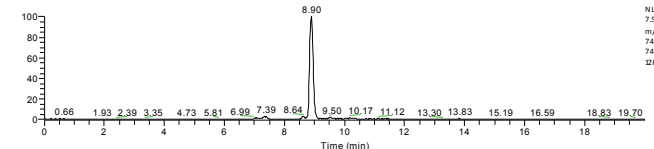
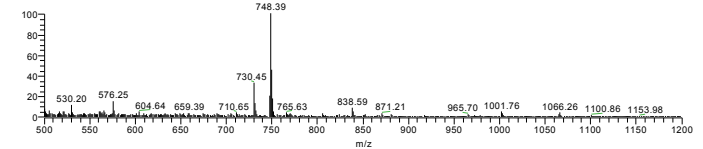
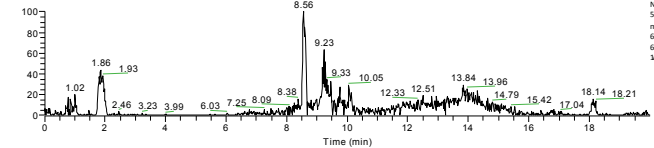
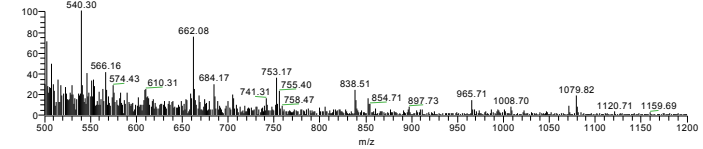
		<p>F:\Other...data\TSPXPFC_96_buz1109H 9/27/2011 11:47:26 PM</p>  <p>Chromatogram peaks (min): 0.84, 2.22, 2.39, 2.54, 4.74, 5.55, 6.75, 6.92, 7.83, 8.25, 10.27, 10.50, 11.50, 12.61, 12.71, 14.27, 15.15, 16.63, 18.69, 19.18</p> <p>Mass spectrum peaks (m/z): 530.62, 563.45, 577.32, 608.29, 676.53, 690.51, 704.58, 718.50, 807.55, 813.50, 835.45, 897.43, 920.23, 1000.53, 1038.54, 1122.80, 1154.07</p> <p>Parameters: NL: 1505.6, m/z: 833.00-834.00, MS 3H</p>
TSEKPC	775	<p>F:\Other...data\TSPXPFC_96_buz1110A 9/28/2011 12:14:30 AM</p>  <p>Chromatogram peaks (min): 0.93, 2.32, 3.34, 4.18, 5.11, 6.96, 7.20, 8.21, 8.56, 8.90, 9.83, 10.53, 11.97, 13.98, 14.69, 16.16, 18.10, 18.77</p> <p>Mass spectrum peaks (m/z): 513.33, 550.89, 576.26, 627.25, 659.28, 689.36, 724.62, 758.47, 775.39, 805.40, 871.14, 907.27, 965.76, 1001.78, 1065.80, 1100.93, 1112.99, 1180.18</p> <p>Parameters: NL: 4.096.6, m/z: 775.00-776.00, MS 3A</p>
TSTSPFC +isoprene	706 774	<p>F:\Other...data\TSPXPFC_96_buz1110E 9/28/2011 2:02:39 AM</p>  <p>Chromatogram peaks (min): 0.04, 1.05, 2.29, 2.61, 4.88, 6.41, 7.20, 7.53, 7.87, 8.59, 8.84, 9.92, 11.66, 12.99, 13.35, 13.81, 14.17, 14.55, 15.13, 15.99, 16.18, 17.19, 18.34</p> <p>Mass spectrum peaks (m/z): 513.58, 550.80, 553.20, 627.33, 659.30, 706.27, 751.45, 758.45, 761.48, 852.68, 926.77, 965.79, 1025.84, 1065.57, 1100.95, 1126.89, 1180.50</p> <p>Parameters: NL: 2256.6, m/z: 706.00-707.00, MS 3E</p> <p>F:\Other...data\TSPXPFC_96_buz1110E 9/28/2011 2:02:39 AM</p>  <p>Chromatogram peaks (min): 0.23, 0.66, 2.32, 2.39, 5.64, 6.63, 7.32, 7.95, 8.00, 9.82, 9.81, 9.86, 10.19, 11.65, 11.94, 13.16, 13.47, 16.15, 16.88, 18.34, 18.67</p> <p>Mass spectrum peaks (m/z): 552.29, 557.91, 576.27, 619.26, 671.41, 704.56, 718.50, 774.41, 807.55, 829.53, 867.66, 930.88, 980.83, 1024.17, 1114.98, 1145.94</p> <p>Parameters: NL: 5.88E.5, m/z: 774.00-775.00, MS 3D</p>

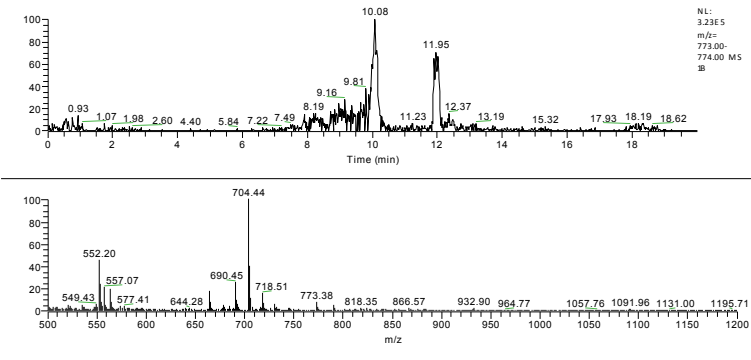
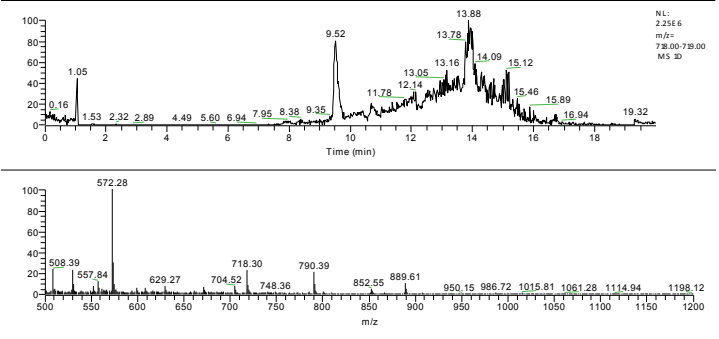
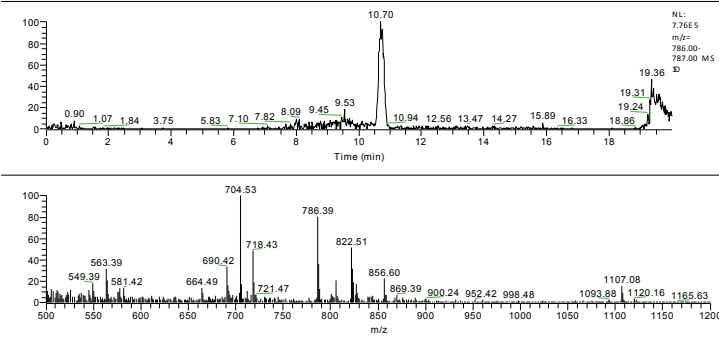
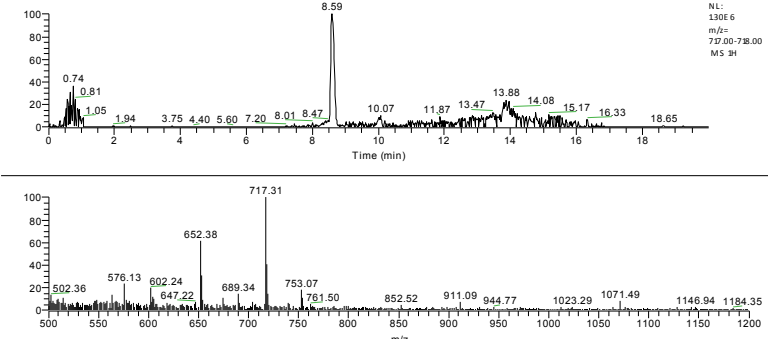
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TSSSPFC	692	<p>F:\Other...data\TSSXPFC_96_buz1110G 9/28/2011 2:56:45 AM</p> <p>Chromatogram Peak: 8.61 min</p> <p>Mass Spectrum Base Peak: 730.39 m/z</p>
TSDGPFC	690	<p>F:\Other...data\TSSXPFC_96_buz1110H 9/28/2011 3:23:45 AM</p> <p>Chromatogram Peak: 13.95 min</p> <p>Mass Spectrum Base Peak: 704.54 m/z</p>
TSASPFC +isoprene	676 744	<p>F:\Other...data\TSSXPFC_96_buz1111B 9/28/2011 4:17:52 AM</p> <p>Chromatogram Peak: 8.73 min</p> <p>Mass Spectrum Base Peak: 676.21 m/z</p>

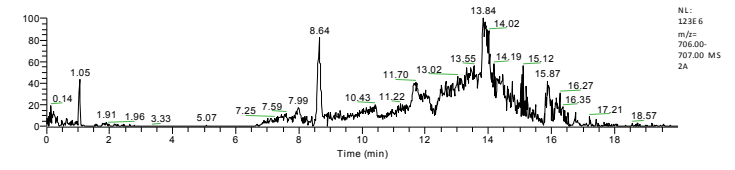
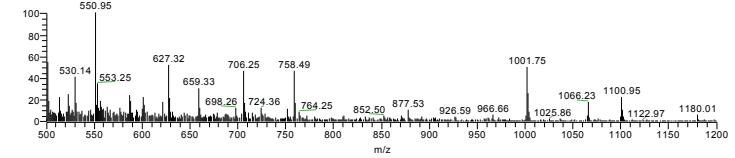
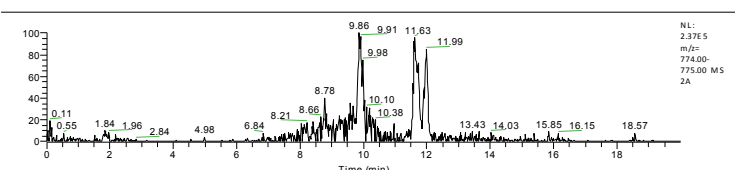
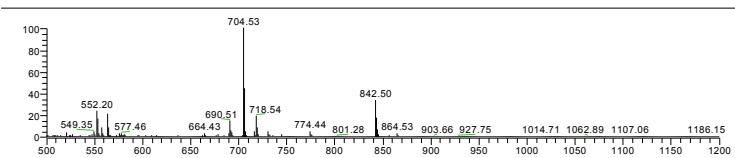
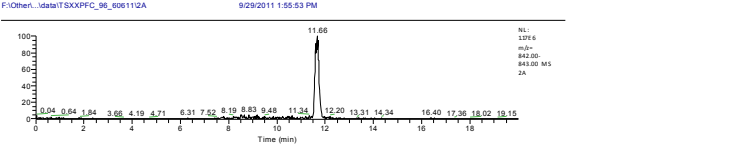
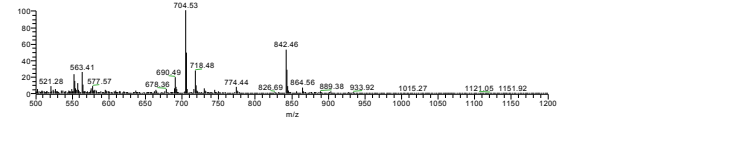
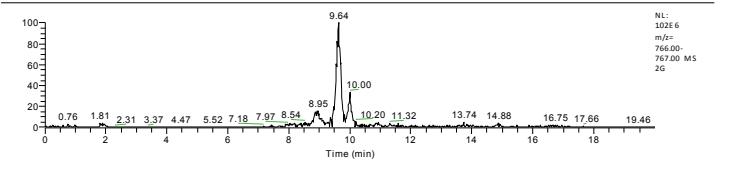
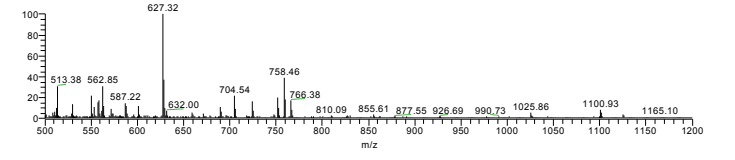
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TSRFPFC	821	<p>F:\Other...data\TSXXPFC_96_buz1111G 9/28/2011 6:33:06 AM</p>
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+isoprene	871	
+2isoprene	939	

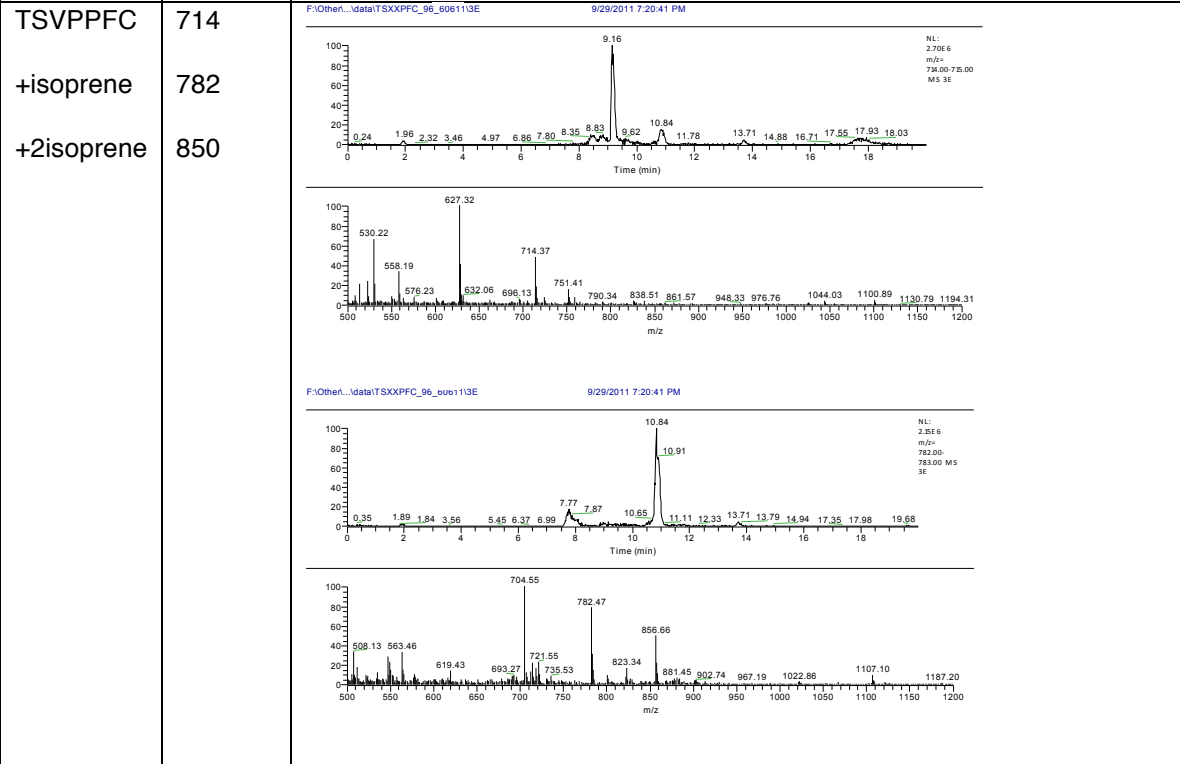
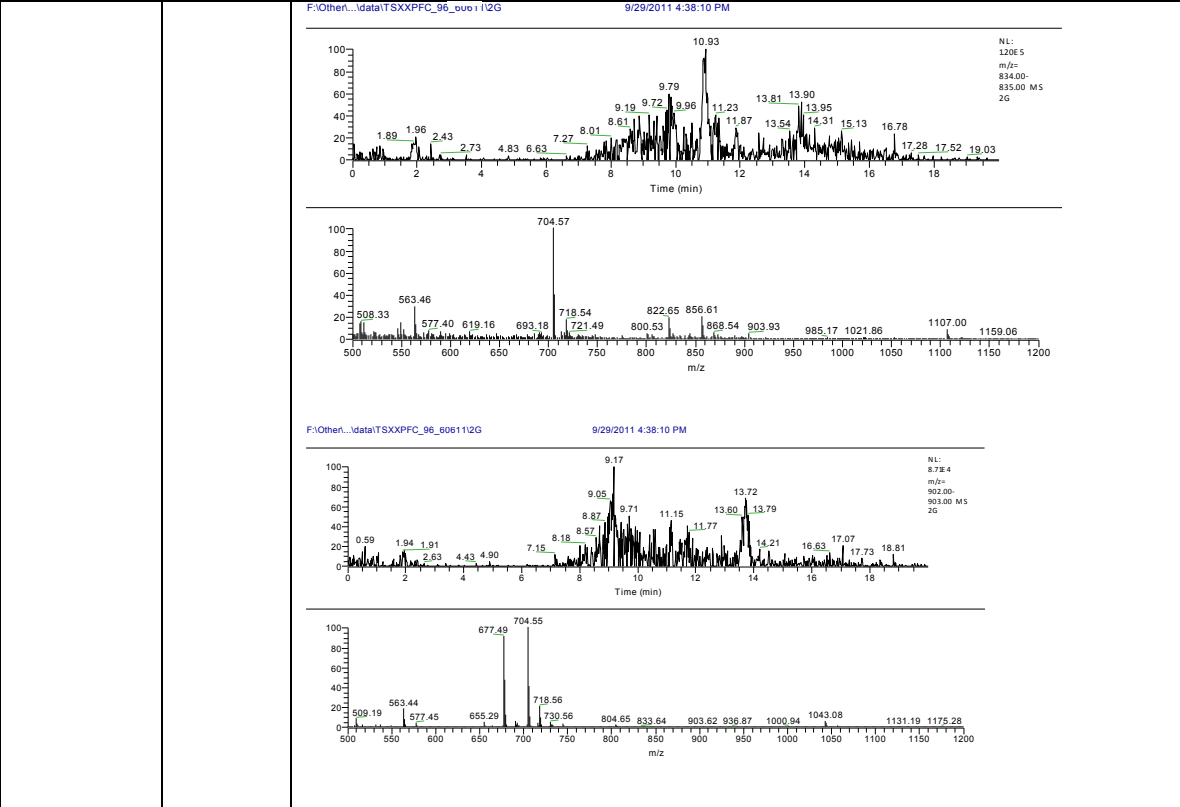
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<p>TSISPC +isoprene +2isoprene</p>	<p>718 786 854</p>	<p>F:\Other_data\TSXXPFC_96_buz11112C 9/28/2011 8:21:15 AM</p>  <p>F:\Other_data\TSXXPFC_96_buz11112C 9/28/2011 8:21:15 AM</p> 

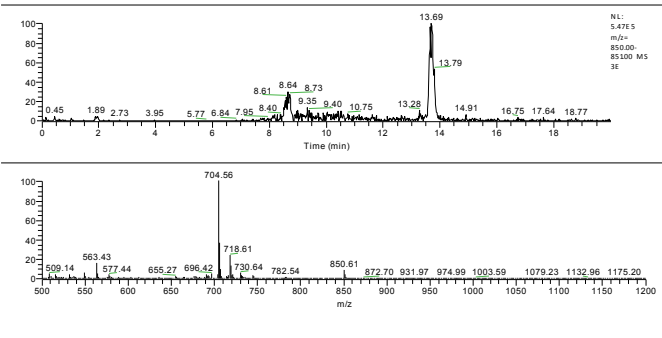
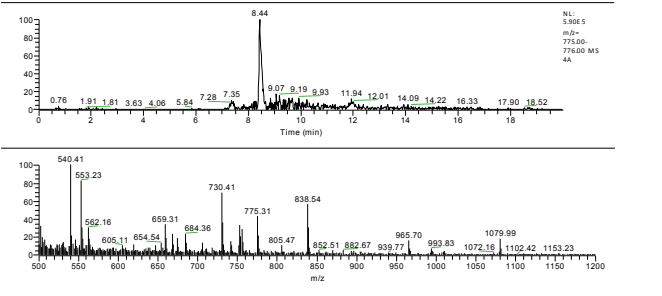
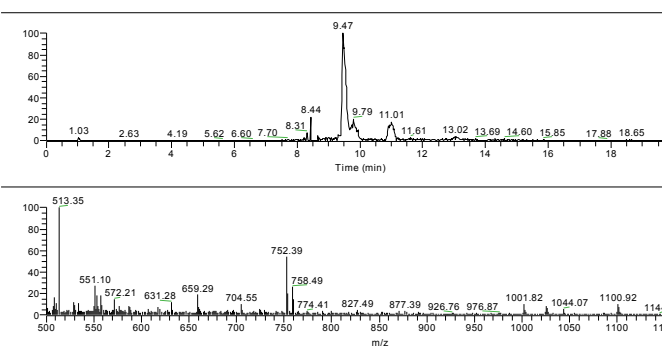
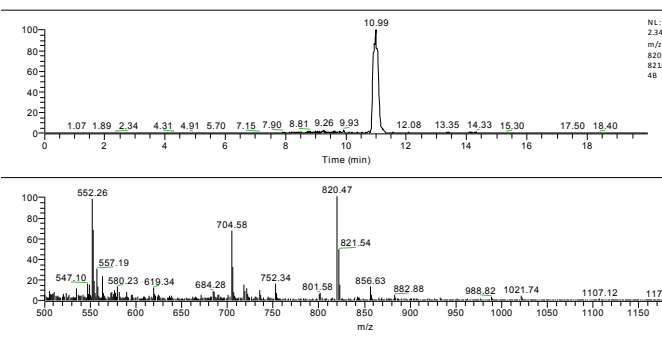
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<p>TSVQFC +isoprene +2isoprene</p>	<p>745 813 881</p>	<p>F:\Other...data\TSXXPFC_96_buz1112D 9/28/2011 8:48:19 AM</p>   <p>F:\Other...data\TSXXPFC_96_buz1112D 9/28/2011 8:48:19 AM</p>   <p>F:\Other...data\TSXXPFC_96_buz1112D 9/28/2011 8:48:19 AM</p>  

<p>TSIQPFC +isoprene</p>	<p>827 895</p>	<p>F:\Other_data\TSXXPFC_96_60z1\112F 9/28/2011 9:42:23 AM</p>  <p>Time (min)</p>  <p>m/z</p> <p>F:\Other_data\TSXXPFC_96_60z1\112F 9/28/2011 9:42:23 AM</p>  <p>Time (min)</p>  <p>m/z</p>
<p>TSETPFC</p>	<p>748</p>	<p>F:\Other_data\TSXXPFC_96_60z1\112H 9/28/2011 10:36:28 AM</p>  <p>Time (min)</p>  <p>m/z</p>
<p>TSGSPFC</p>	<p>662</p>	<p>F:\Other_data\TSXXPFC_96_60b1\111A 9/29/2011 10:19:31 AM</p>  <p>Time (min)</p>  <p>m/z</p>

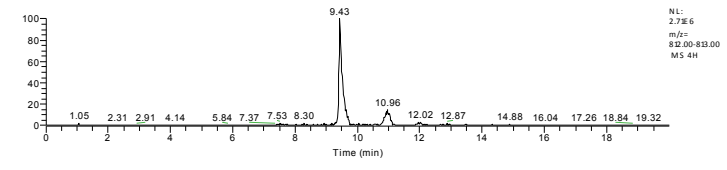
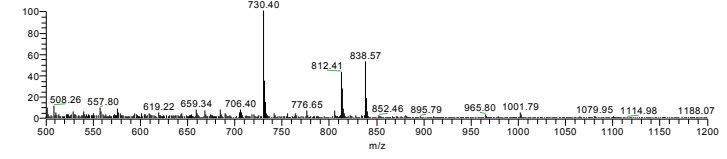
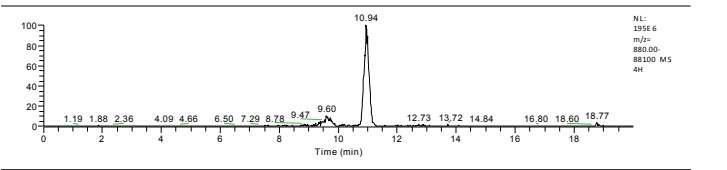
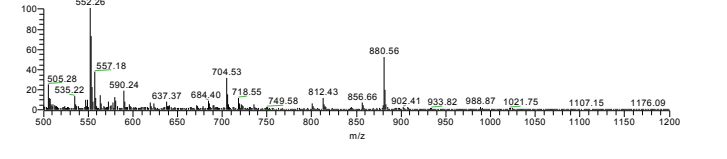
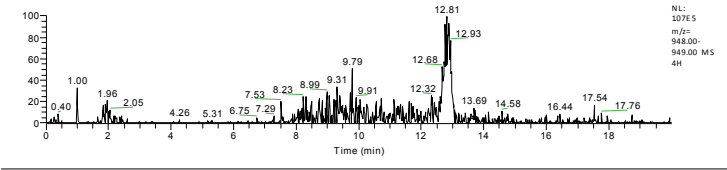
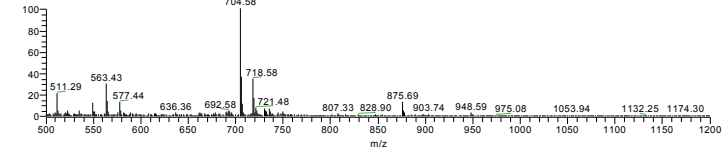
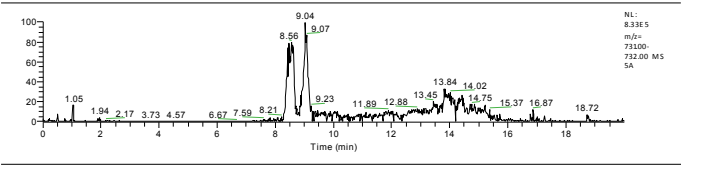
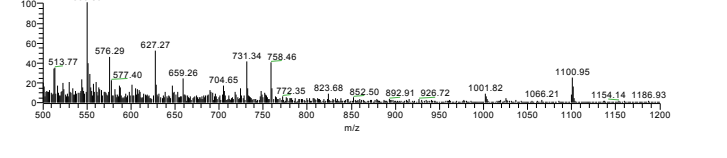
TSRVPCF	773	<p>F:\Other...data\TSXXPCF_96_006111B 9/29/2011 10:46:33 AM</p>  <p>Chromatogram (Time (min) vs. Intensity) showing peaks at 10.08 and 11.95. Mass spectrum (m/z vs. Intensity) showing peaks at 552.20, 704.44, and 718.51.</p>
TSSLPCF +isoprene	718 786	<p>F:\Other...data\TSXXPCF_96_006111D 9/29/2011 11:40:39 AM</p>  <p>Chromatogram (Time (min) vs. Intensity) showing peaks at 9.52, 13.78, and 13.88. Mass spectrum (m/z vs. Intensity) showing peaks at 572.28, 718.30, and 790.39.</p> <p>F:\Other...data\TSXXPCF_96_006111D 9/29/2011 11:40:39 AM</p>  <p>Chromatogram (Time (min) vs. Intensity) showing a major peak at 10.70. Mass spectrum (m/z vs. Intensity) showing peaks at 704.53, 786.39, and 822.51.</p>
TSQAPCF	717	<p>F:\Other...data\TSXXPCF_96_006111H 9/29/2011 1:28:53 PM</p>  <p>Chromatogram (Time (min) vs. Intensity) showing a major peak at 8.59. Mass spectrum (m/z vs. Intensity) showing peaks at 652.38, 717.31, and 753.07.</p>

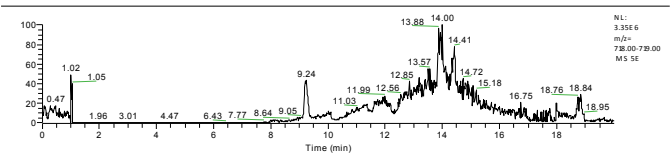
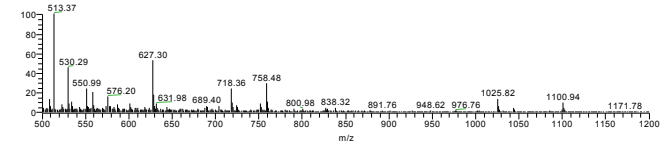
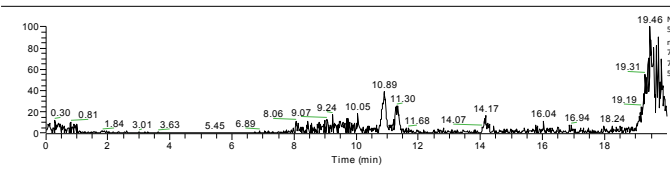
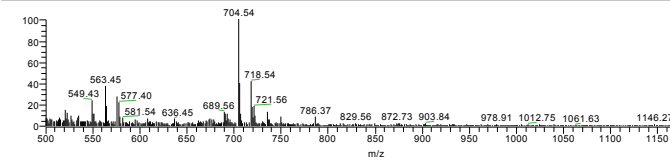
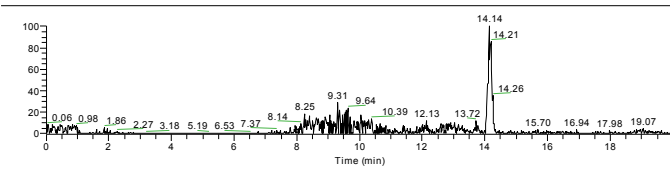
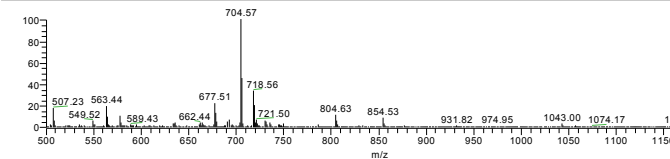
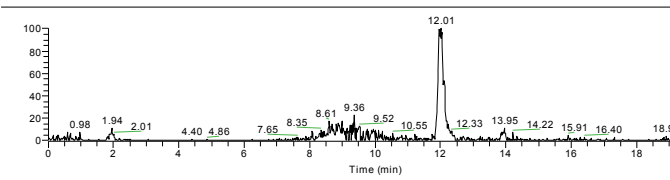
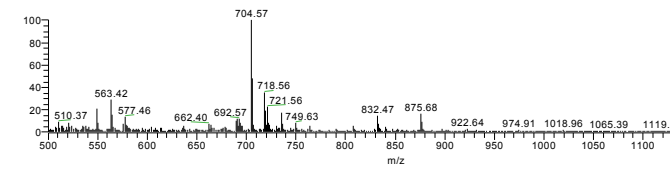
<p>TSTSPFC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>706</p> <p>774</p> <p>842</p>	<p>F:\Other...data\TSTSPFC_96_6061102A 9/29/2011 1:55:53 PM</p>  <p>Chromatogram showing peaks at 8.64, 13.84, 14.02, 14.19, 15.12, 15.87, 16.27, 16.35, 17.21, 18.57. NL: 12366, m/z: 706.00-707.00 MS 2A.</p>  <p>Mass spectrum showing major peak at 550.95. Other peaks at 530.14, 553.25, 627.32, 659.33, 698.26, 706.25, 724.36, 758.49, 764.25, 852.59, 877.53, 926.59, 966.66, 1001.75, 1066.23, 1100.95, 1122.97, 1180.01.</p> <p>F:\Other...data\TSTSPFC_96_6061102A 9/29/2011 1:55:53 PM</p>  <p>Chromatogram showing peaks at 9.86, 9.91, 11.63, 11.99, 13.43, 14.03, 15.85, 16.15, 18.57. NL: 23765, m/z: 774.00-775.00 MS 2A.</p>  <p>Mass spectrum showing major peak at 704.53. Other peaks at 549.35, 552.20, 577.46, 664.43, 690.51, 718.54, 774.44, 801.28, 842.50, 864.53, 903.66, 927.75, 1014.71, 1062.89, 1107.06, 1186.15.</p> <p>F:\Other...data\TSTSPFC_96_6061102A 9/29/2011 1:55:53 PM</p>  <p>Chromatogram showing major peak at 11.66. NL: 12916, m/z: 842.00-843.00 MS 2A.</p>  <p>Mass spectrum showing major peak at 704.53. Other peaks at 553.41, 577.57, 690.49, 674.36, 718.48, 774.44, 826.89, 842.46, 864.56, 889.38, 933.92, 1015.27, 1121.65, 1151.92.</p>
<p>TSTFPFC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>766</p> <p>834</p> <p>902</p>	<p>F:\Other...data\TSTFPFC_96_6061102G 9/29/2011 4:38:10 PM</p>  <p>Chromatogram showing peaks at 9.64, 10.00, 10.20, 11.32, 13.74, 14.88, 16.75, 17.66, 19.46. NL: 102E6, m/z: 766.00-767.00 MS 2G.</p>  <p>Mass spectrum showing major peak at 627.32. Other peaks at 513.38, 562.85, 587.22, 632.00, 704.54, 758.46, 768.38, 810.09, 855.61, 877.55, 926.69, 990.73, 1025.86, 1100.93, 1165.10.</p>



		<p>F:\Other...data\TSXXPFC_96_sub113E 9/29/2011 7:20:41 PM</p>  <p>Chromatogram peaks (min): 0.45, 1.89, 2.73, 3.95, 5.77, 6.84, 7.95, 8.40, 8.61, 8.64, 8.73, 9.35, 9.40, 10.75, 13.28, 13.69, 14.91, 16.75, 17.64, 18.77</p> <p>Mass spectrum peaks (m/z): 509.14, 563.43, 577.44, 655.27, 696.42, 704.56, 715.61, 730.64, 782.54, 850.61, 872.70, 931.97, 974.99, 1003.59, 1079.23, 1132.96, 1175.20</p> <p>Parameters: NL: 5.47E5, m/z: 850.00, 85.00 MS, 3E</p>
TSQEPFC	775	<p>F:\Other...data\TSXXPFC_96_sub114A 9/29/2011 9:08:49 PM</p>  <p>Chromatogram peaks (min): 0.76, 1.91, 1.81, 3.63, 4.06, 5.84, 7.28, 7.35, 8.44, 9.07, 9.19, 9.93, 11.94, 12.01, 14.09, 14.22, 16.33, 17.90, 18.52</p> <p>Mass spectrum peaks (m/z): 540.41, 553.33, 562.16, 605.11, 654.54, 659.31, 684.36, 730.41, 775.31, 805.47, 838.54, 852.51, 882.67, 939.77, 965.70, 995.83, 1072.16, 1079.99, 1102.42, 1153.23</p> <p>Parameters: NL: 5.90E5, m/z: 775.00, 776.00 MS, 4A</p>
TSFSPFC	752	<p>F:\Other...data\TSXXPFC_96_sub114B 9/29/2011 9:35:53 PM</p>  <p>Chromatogram peaks (min): 1.03, 2.63, 4.19, 5.62, 6.60, 7.70, 8.31, 8.44, 9.47, 9.79, 11.01, 11.61, 13.02, 13.69, 14.60, 15.85, 17.88, 18.65</p> <p>Mass spectrum peaks (m/z): 513.35, 551.10, 572.21, 631.28, 659.29, 704.55, 752.39, 758.49, 774.41, 827.49, 877.39, 926.76, 976.87, 1001.82, 1044.07, 1100.92, 1144.13, 1185.23</p> <p>Parameters: NL: 2.30E6, m/z: 752.00, 753.00 MS, 4B</p> <p>F:\Other...data\TSXXPFC_96_sub114B 9/29/2011 9:35:53 PM</p>  <p>Chromatogram peaks (min): 1.07, 1.89, 2.34, 4.31, 4.91, 5.70, 7.15, 7.90, 8.81, 9.26, 9.93, 10.99, 12.08, 13.35, 14.33, 15.30, 17.50, 18.40</p> <p>Mass spectrum peaks (m/z): 547.10, 552.26, 557.19, 590.23, 619.34, 684.28, 704.58, 752.34, 801.58, 820.47, 821.54, 856.63, 882.88, 988.82, 1021.74, 1107.12, 1176.76</p> <p>Parameters: NL: 2.34E6, m/z: 820.00, 821.00 MS, 4B</p>

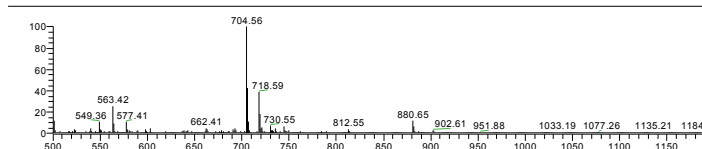
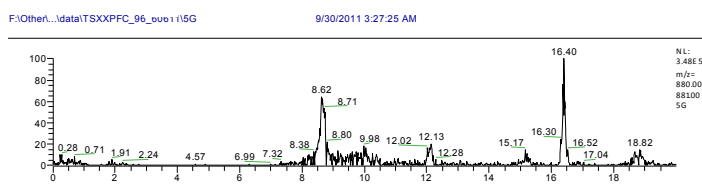
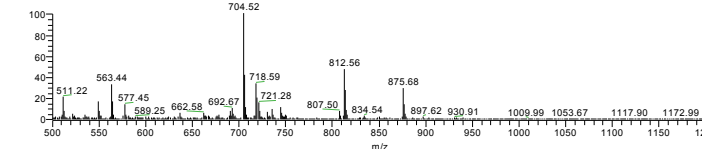
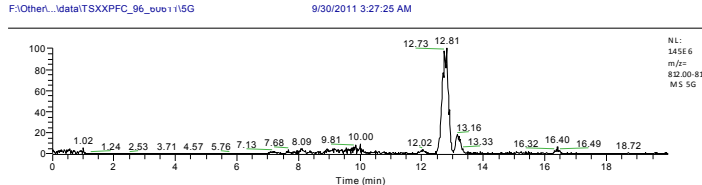
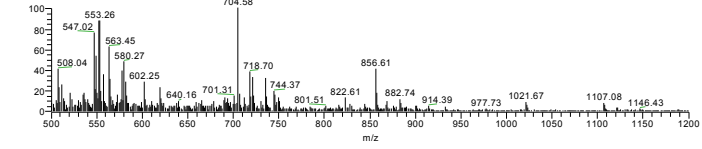
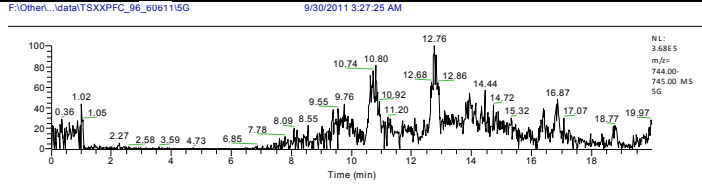
<p>TSQAPFC</p>	<p>717</p>	<p>F:\Other...data\TSXXPFC_96_00e114C 9/29/2011 10:02:55 PM</p> <p>Chromatogram (Time (min)) peaks: 0.40, 1.58, 2.29, 2.37, 4.59, 5.29, 7.03, 7.94, 8.38, 8.57, 9.77, 10.12, 11.82, 13.81, 13.91, 14.70, 16.78, 17.11, 18.36</p> <p>Mass Spectrum (m/z) peaks: 540.23, 562.14, 617.33, 674.37, 717.33, 730.41, 739.39, 805.48, 838.55, 890.69, 907.07, 965.83, 1001.78, 1065.84, 1121.48, 1159.33</p> <p>Metadata: NL: 9.66E5, m/z: 717.00, MS: 4C</p>
<p>TSTTPFC</p>	<p>720</p>	<p>F:\Other...data\TSXXPFC_96_00e114F 9/29/2011 11:24:04 PM</p> <p>Chromatogram (Time (min)) peaks: 1.05, 2.27, 3.03, 4.02, 4.69, 7.10, 8.18, 8.57, 8.74, 8.95, 9.50, 12.80, 13.79, 13.91, 14.32, 15.10, 16.76, 18.02, 19.56</p> <p>Mass Spectrum (m/z) peaks: 513.08, 550.94, 553.27, 562.12, 617.27, 631.41, 659.41, 720.30, 758.50, 765.59, 805.48, 838.58, 871.33, 907.10, 965.82, 1001.84, 1065.90, 1100.99, 1173.02, 1180.31</p> <p>Metadata: NL: 1.87E6, m/z: 720.00, MS: 4F</p>
<p>TSFLPFC +isoprene</p>	<p>778 846</p>	<p>F:\Other...data\TSXXPFC_96_00e114G 9/29/2011 11:51:06 PM</p> <p>Chromatogram (Time (min)) peaks: 1.03, 1.96, 2.85, 3.25, 4.57, 5.05, 7.22, 7.80, 9.12, 9.81, 10.36, 10.77, 11.04, 12.62, 13.98, 14.10, 16.56, 18.31, 18.69</p> <p>Mass Spectrum (m/z) peaks: 508.00, 553.48, 577.43, 619.23, 692.54, 704.56, 718.58, 749.72, 778.43, 822.48, 856.63, 867.57, 903.63, 945.08, 1021.77, 1067.58, 1107.10, 1158.16</p> <p>Metadata: NL: 8.59E5, m/z: 778.00, MS: 4G</p> <p>F:\Other...data\TSXXPFC_96_00e114G 9/29/2011 11:51:06 PM</p> <p>Chromatogram (Time (min)) peaks: 1.03, 1.96, 2.44, 4.42, 4.85, 6.44, 7.80, 8.47, 9.17, 9.91, 10.92, 12.00, 12.68, 13.14, 15.10, 16.68, 17.16, 18.12, 19.17</p> <p>Mass Spectrum (m/z) peaks: 511.19, 563.42, 577.46, 636.44, 692.52, 704.57, 718.61, 778.46, 807.46, 846.56, 875.66, 903.66, 936.69, 964.94, 1023.84, 1082.17, 1121.11, 1173.28</p> <p>Metadata: NL: 2.46E6, m/z: 846.00, MS: 4G</p>

<p>TSMYPFC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>812</p> <p>880</p> <p>948</p>	<p>F:\Other...data\TSMYPFC_96_bu06114H 9/30/2011 12:18:06 AM</p>  <p>NL: 2.7E6 m/z: 812.00-813.00 MS 4H</p>  <p>F:\Other...data\TSMYPFC_96_bu06114H 9/30/2011 12:18:06 AM</p>  <p>NL: 1.95E6 m/z: 880.00-88100 MS 4H</p>  <p>F:\Other...data\TSMYPFC_96_bu06114H 9/30/2011 12:18:06 AM</p>  <p>NL: 1.07E5 m/z: 948.00-949.00 MS 4H</p> 
<p>TSNVPFC</p>	<p>731</p>	<p>F:\Other...data\TSNVPFC_96_bu061115A 9/30/2011 12:45:10 AM</p>  <p>NL: 8.33E5 m/z: 731.00-732.00 MS 5A</p> 

<p>TSVTPFC</p> <p>+isoprene</p> <p>+2isoprene</p>	<p>718</p> <p>786</p> <p>854</p>	<p>F:\Other...data\TSXXPFC_96_bu6111SE 9/30/2011 2:33:19 AM</p>   <p>F:\Other...data\TSXXPFC_96_bu6111SE 9/30/2011 2:33:19 AM</p>   <p>F:\Other...data\TSXXPFC_96_bu6111SE 9/30/2011 2:33:19 AM</p>  
<p>TSFVPFC</p> <p>+isoprene</p>	<p>832</p>	<p>F:\Other...data\TSXXPFC_96_bu6111SF 9/30/2011 3:00:21 AM</p>  

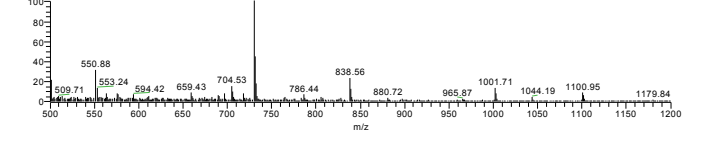
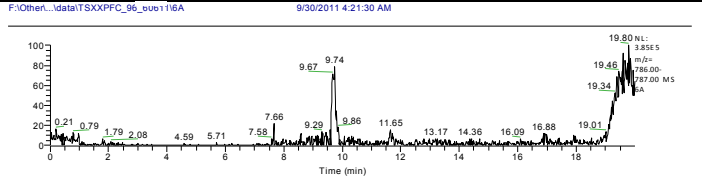
TSIIPFC
 +isoprene
 +2isoprene

744
 812
 880



TSAEPFC
 +isoprene
 +2isoprene

786
 854

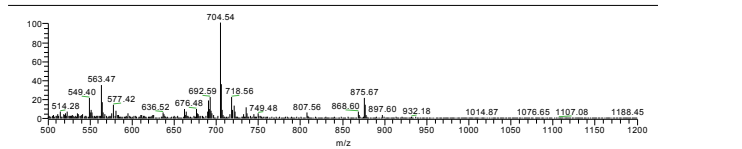
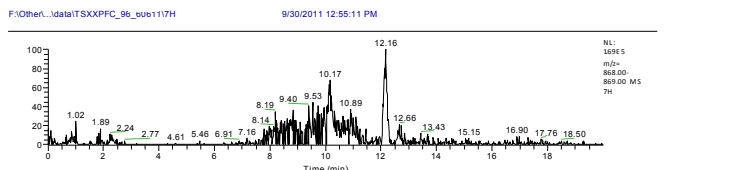
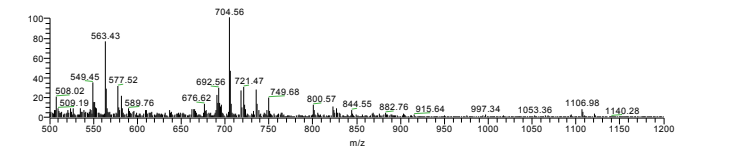
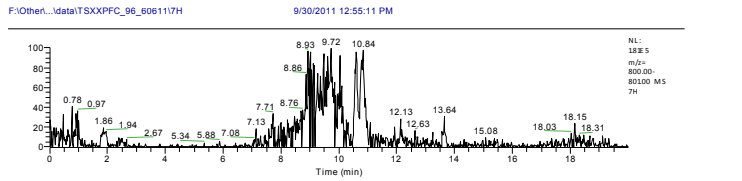
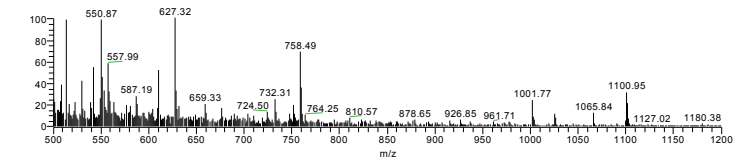
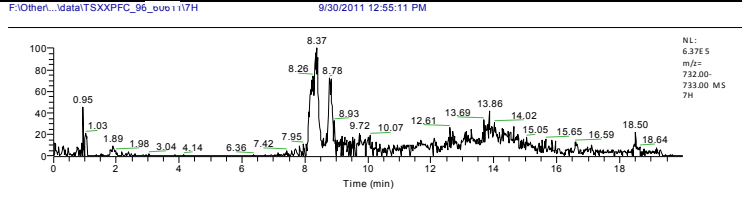


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TSQGFC	703	<p>F:\Other_data\TSXXPFC_06_bue1117C 9/30/2011 10:39:56 AM</p>
TSMFPFC	778	<p>F:\Other_data\TSXXPFC_06_bue1117E 9/30/2011 11:34:03 AM</p>

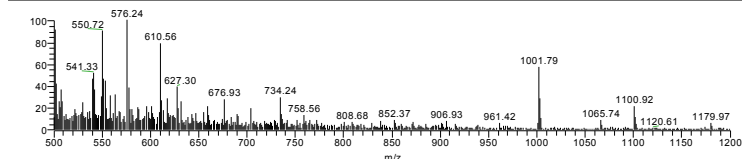
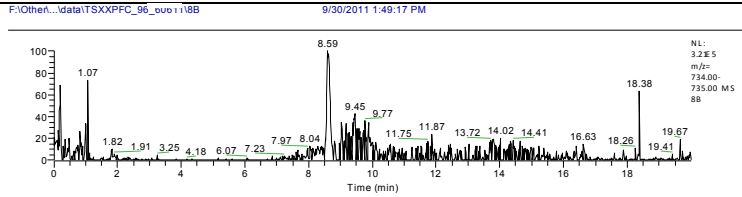
TSVDFPC 732

+isoprene 800

+2isoprene 868

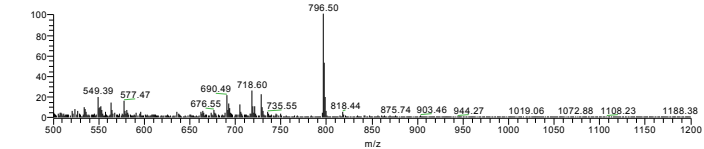
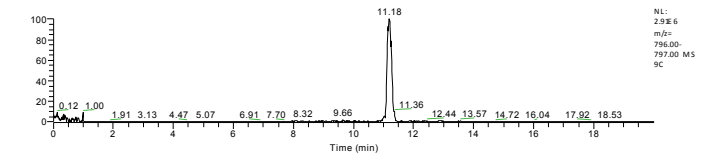


TSESPFC 734

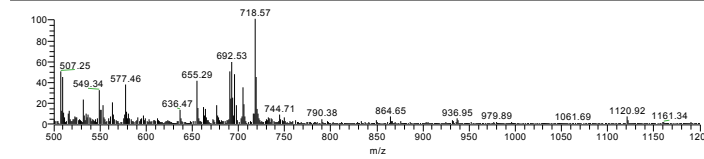
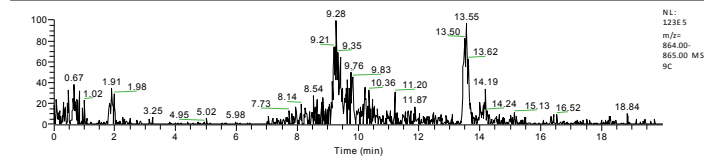


TSRYPFC	837	<p>F:\Other...data\TSXXPFC_96_u06118E 9/30/2011 3:10:46 PM</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 3.97E5 m/z: 837.00 838.00 MS 8E</p>
TSEFPFC	794	<p>F:\Other...data\TSXXPFC_96_u06118G 9/30/2011 4:04:52 PM</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 2.5E6 m/z: 794.00 795.00 MS 8G</p>
TSSSPFC +2isoprene	828	<p>F:\Other...data\TSXXPFC_96_u06119A 9/30/2011 4:58:58 PM</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 1.66E5 m/z: 828.00 829.00 MS 9A</p>
TSLPPFC +isoprene +2isoprene	729 796 864	<p>F:\Other...data\TSXXPFC_96_u06119C 9/30/2011 5:53:01 PM</p> <p>Time (min)</p> <p>m/z</p> <p>NL: 3.07E6 m/z: 728.00 729.00 MS 9C</p>

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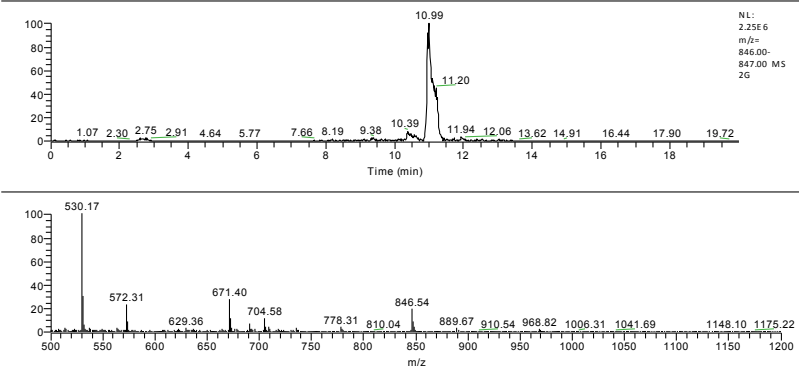
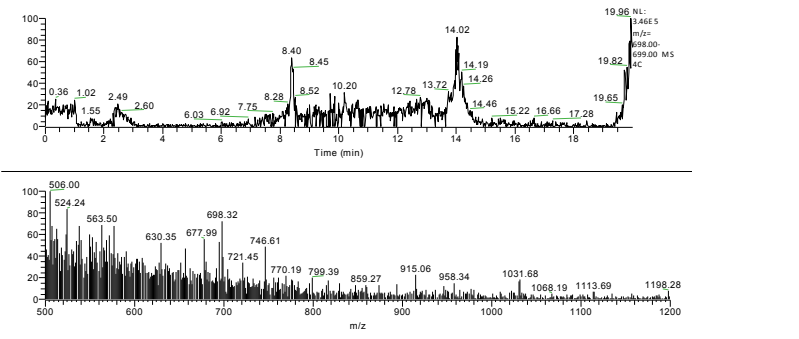
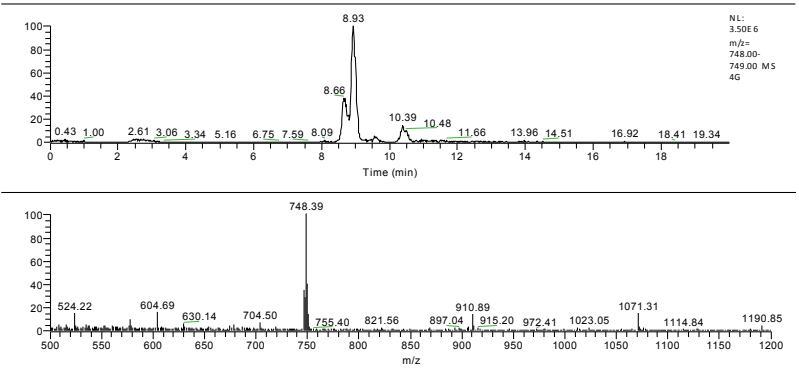


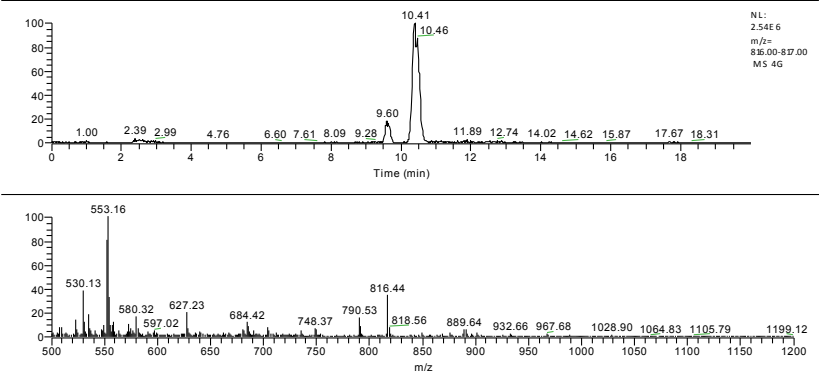
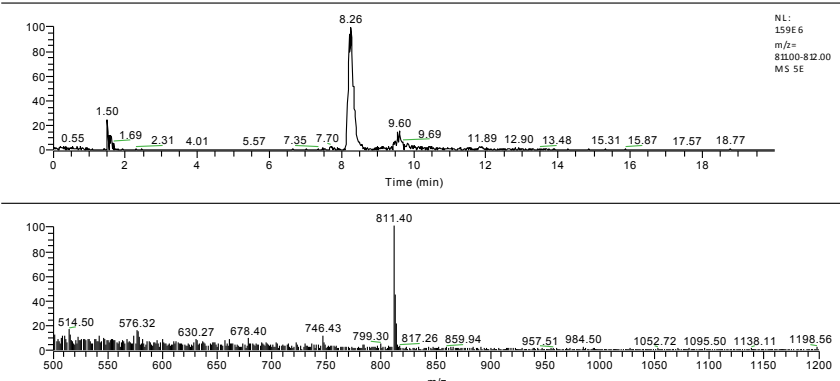
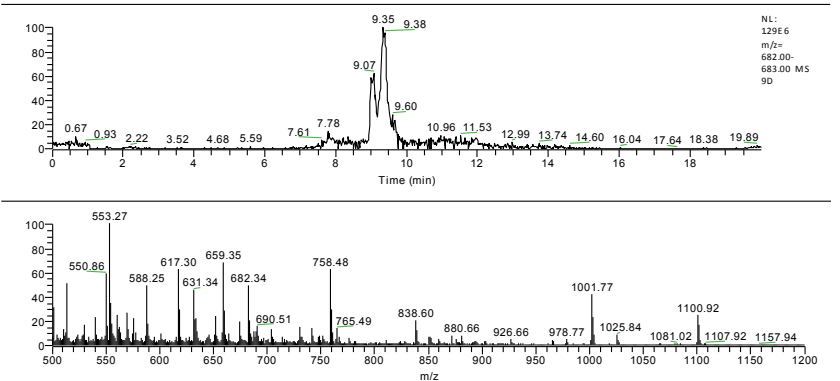
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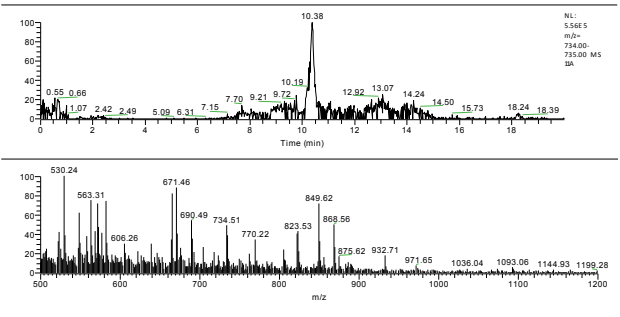
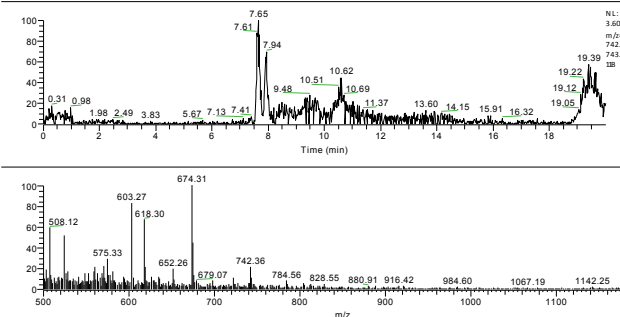


S4D. XSXXPXC

Sequence	m/z	Extracted ion chromatogram and mass spectrum at time point
DSEVPTC (+isoprene)	782	<p>F:\Other...data\XSXXPXC_96_12091111G 12/8/2011 6:44:00 PM</p> <p>Chromatogram peaks (min): 0.69, 0.78, 2.70, 2.91, 4.68, 6.13, 7.77, 8.30, 8.45, 8.61, 8.66, 8.80, 9.23, 10.10, 10.67, 11.46, 12.01, 13.04, 13.79, 16.64, 17.38, 19.20</p> <p>Mass spectrum peaks (m/z): 553.35, 577.38, 652.32, 668.39, 746.30, 782.42, 821.62, 856.62, 883.60, 940.10, 966.63, 1028.06, 1084.10, 1172.00</p>
TSYAPWC	791	<p>F:\Other...data\XSXXPXC_96_12091112B 12/8/2011 8:05:02 PM</p> <p>Chromatogram peaks (min): 0.97, 1.07, 2.39, 2.96, 5.09, 7.25, 8.16, 8.31, 9.16, 9.28, 9.47, 10.96, 11.27, 12.26, 13.90, 13.91, 14.00, 14.17, 15.44, 16.83, 18.89, 19.12</p> <p>Mass spectrum peaks (m/z): 523.52, 589.18, 630.21, 651.70, 704.47, 715.87, 753.08, 791.33, 828.98, 892.98, 943.26, 980.94, 1065.94, 1047.23, 1073.21, 1172.76</p>
YSTIPMC (+isoprene)	778	<p>F:\Other...data\XSXXPXC_96_12091112G 12/8/2011 10:20:07 PM</p> <p>Chromatogram peaks (min): 0.74, 0.97, 2.77, 2.94, 5.12, 6.46, 7.25, 7.89, 8.93, 9.24, 9.36, 9.60, 10.98, 11.08, 13.90, 14.46, 16.28, 17.88, 18.69</p> <p>Mass spectrum peaks (m/z): 540.35, 575.31, 651.93, 674.26, 704.55, 753.40, 778.37, 794.44, 862.49, 915.91, 907.30, 965.79, 1008.91, 1079.87, 1110.87, 1180.08</p>

		<p>F:\Other...data\XSSXPXC_96_12091112G 12/8/2011 10:20:07 PM</p>  <p>Chromatogram peaks (min): 1.07, 2.30, 2.75, 2.91, 4.64, 5.77, 7.66, 8.19, 9.38, 10.39, 10.99, 11.20, 11.94, 12.06, 13.62, 14.91, 16.44, 17.90, 19.72</p> <p>Mass spectrum peaks (m/z): 530.17, 572.31, 629.36, 671.40, 704.58, 778.31, 810.04, 846.54, 889.67, 910.54, 968.82, 1006.31, 1041.69, 1148.10, 1175.22</p> <p>Parameters: NL: 2.25E6, m/z: 846.00-847.00 MS, 2G</p>
ESADPLC	698	<p>F:\Other...data\XSSXPXC_96_12091114C 12/9/2011 11:51:11 AM</p>  <p>Chromatogram peaks (min): 0.36, 1.02, 1.55, 2.49, 2.60, 6.03, 6.92, 7.75, 8.28, 8.40, 8.45, 8.52, 10.20, 12.78, 13.72, 14.02, 14.19, 14.26, 14.46, 15.22, 16.66, 17.28, 19.65, 19.82</p> <p>Mass spectrum peaks (m/z): 506.00, 524.24, 563.50, 630.35, 677.99, 698.32, 746.61, 721.45, 770.19, 799.39, 859.27, 915.06, 958.34, 1031.68, 1068.19, 1113.69, 1198.28</p> <p>Parameters: NL: 1.46E5, m/z: 698.00-699.00 MS, 1G</p>
YSTTPLC (+isoprene)	748 816	<p>F:\Other...data\XSSXPXC_96_12091114G 12/9/2011 1:39:12 PM</p>  <p>Chromatogram peaks (min): 0.43, 1.00, 2.61, 3.06, 3.34, 5.16, 6.75, 7.59, 8.09, 8.66, 8.93, 10.39, 10.48, 11.66, 13.96, 14.51, 16.92, 18.41, 19.34</p> <p>Mass spectrum peaks (m/z): 524.22, 604.69, 630.14, 704.50, 748.39, 755.40, 821.56, 897.04, 910.89, 915.20, 972.41, 1023.05, 1071.31, 1114.84, 1190.85</p> <p>Parameters: NL: 3.50E6, m/z: 748.00-749.00 MS, 4G</p>

		<p>F:\Other...data\XSPXPC_96_1209114G 12/9/2011 1:39:12 PM</p>  <p>Chromatogram peaks (min): 1.00, 2.39, 2.99, 4.76, 6.60, 7.61, 8.09, 9.28, 9.60, 10.41, 10.46, 11.89, 12.74, 14.02, 14.62, 15.87, 17.67, 18.31</p> <p>Mass spectrum peaks (m/z): 530.13, 553.16, 580.32, 597.02, 627.23, 684.42, 748.37, 790.53, 816.44, 818.56, 889.64, 932.66, 967.68, 1028.90, 1064.83, 1105.79, 1199.12</p> <p>Parameters: NL: 2.54E 6, m/z: 816.00-817.00, MS 4G</p>
WSNLPQC	811	<p>F:\Other...data\XSPXPC_96_1209115E 12/9/2011 4:21:15 PM</p>  <p>Chromatogram peaks (min): 0.55, 1.50, 1.69, 2.31, 4.01, 5.57, 7.35, 7.70, 8.26, 9.60, 9.69, 11.89, 12.90, 13.48, 15.31, 15.87, 17.57, 18.77</p> <p>Mass spectrum peaks (m/z): 514.50, 576.32, 630.27, 678.40, 746.43, 799.30, 811.40, 817.26, 859.94, 957.51, 984.50, 1052.72, 1095.50, 1138.11, 1198.56</p> <p>Parameters: NL: 1.59E 6, m/z: 811.00-812.00, MS 5E</p>
VSEAPLC	682	<p>F:\Other...data\XSPXPC_96_1209119D 12/12/2011 6:32:45 PM</p>  <p>Chromatogram peaks (min): 0.67, 0.93, 2.22, 3.52, 4.68, 5.59, 7.61, 7.78, 9.07, 9.35, 9.38, 9.60, 10.96, 11.53, 12.99, 13.74, 14.60, 16.04, 17.64, 18.38, 19.89</p> <p>Mass spectrum peaks (m/z): 550.86, 553.27, 588.25, 617.30, 631.34, 659.35, 682.34, 690.51, 758.48, 765.49, 838.60, 880.66, 926.66, 978.77, 1001.77, 1025.84, 1100.92, 1081.02, 1107.92, 1157.94</p> <p>Parameters: NL: 1.29E 6, m/z: 682.00-683.00, MS 9D</p>

<p>HSTIPLC</p>	<p>734</p>	<p>F:\Other...data\XSSXPXC_96_12091111A 12/13/2011 2:43:38 PM</p>  <p>Chromatogram peaks (min): 0.55, 0.66, 1.07, 2.42, 2.49, 5.09, 6.31, 7.15, 7.70, 9.21, 9.72, 10.38, 12.82, 13.07, 14.24, 14.60, 15.73, 18.24, 18.39.</p> <p>Mass spectrum peaks (m/z): 530.24, 563.31, 606.26, 671.46, 690.49, 734.51, 770.22, 823.53, 849.62, 868.56, 875.62, 932.71, 971.65, 1036.04, 1093.06, 1144.93, 1199.28.</p> <p>Metadata: NL: 3.56E5, m/z: 734.00, 735.00 MS, DA</p>
<p>QSWGPTC</p>	<p>742</p>	<p>F:\Other...data\XSSXPXC_96_12091111B 12/13/2011 3:10:38 PM</p>  <p>Chromatogram peaks (min): 0.31, 0.98, 1.98, 2.49, 3.83, 5.67, 7.13, 7.41, 7.65, 7.61, 7.94, 9.48, 10.51, 10.62, 10.69, 11.37, 13.60, 14.15, 15.91, 16.32, 19.05, 19.12, 19.22, 19.39.</p> <p>Mass spectrum peaks (m/z): 508.12, 575.33, 603.27, 618.30, 652.26, 674.31, 679.07, 742.36, 784.56, 828.55, 880.91, 916.42, 984.60, 1067.19, 1142.25, 1194.20.</p> <p>Metadata: NL: 3.60E5, m/z: 742.00, 743.00 MS, DA</p>