

Data Path : C:\msdchem\1\LEGACY\2012\February\  
Data File : 020312PA--Day8-1mL.D  
Acq On : 3 Feb 2012 8:54  
Operator :  
Sample : PA--Day8-1mL  
Misc : 1 uL PA--Day8 at 1 mL  
ALS Vial : 92 Sample Multiplier: 1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : C:\msdchem\1\METHODS\TLTICPAH.M

Title : PAH5437

Signal : TIC: 020312PA--Day8-1mL.D\data.ms

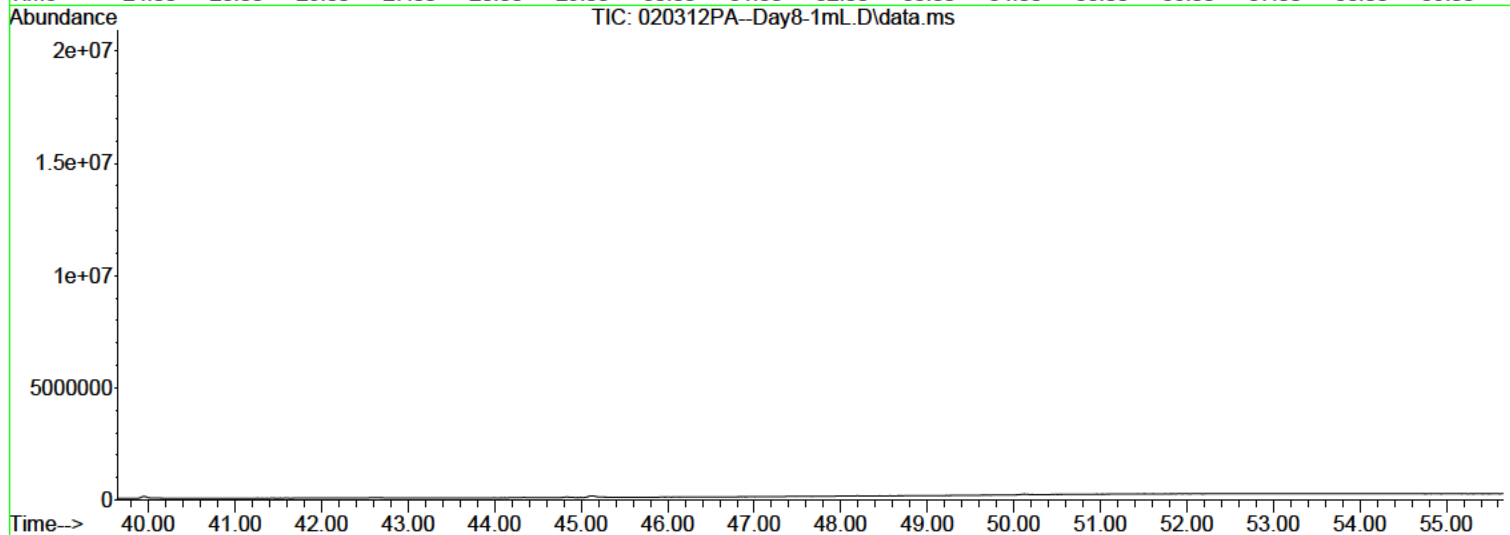
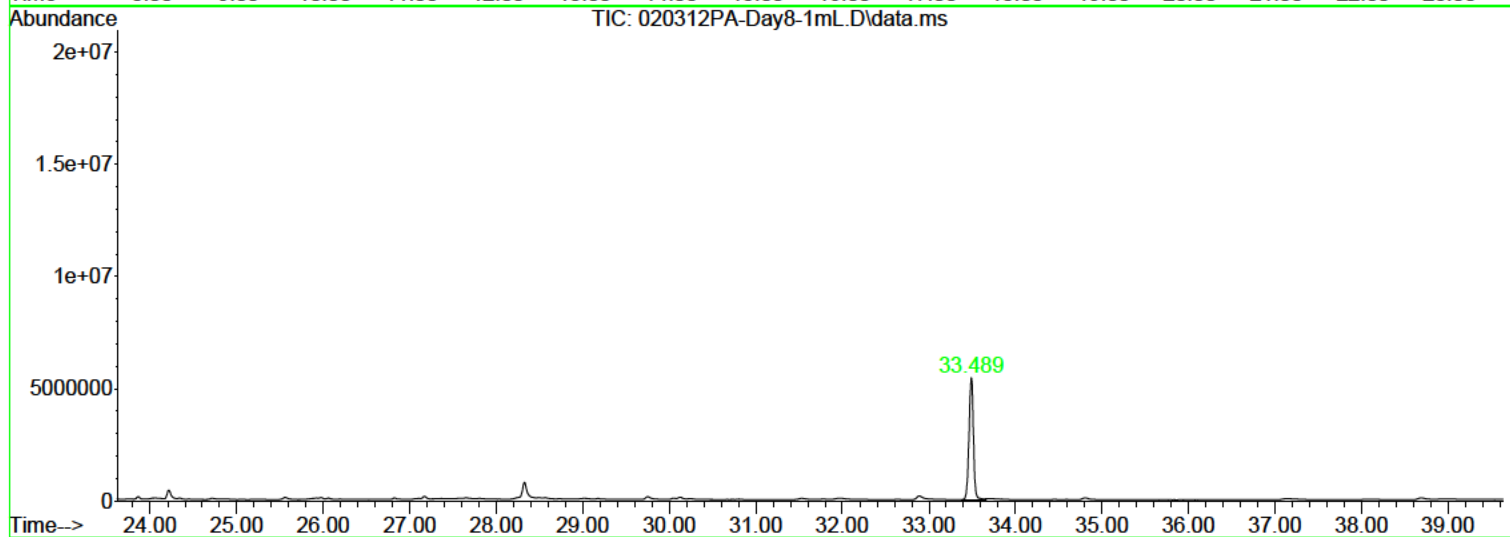
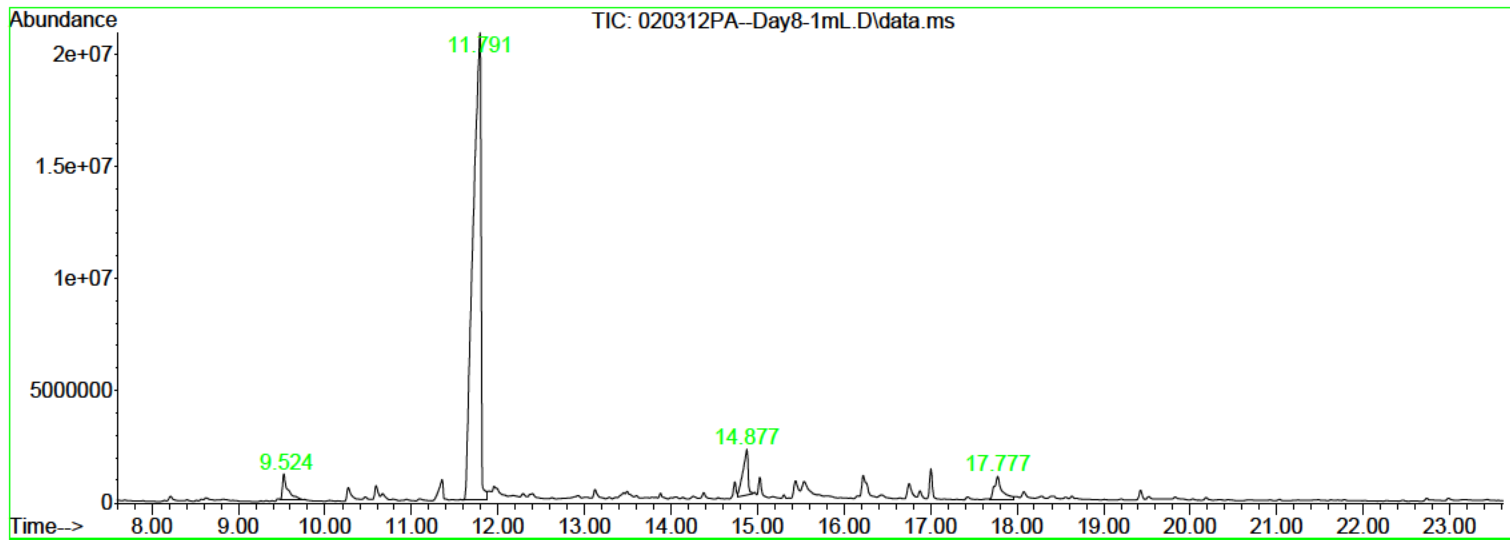
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1	9.524	406	415	463	rVB2	1145754	4739530	3.58%	2.770%
2	11.791	861	902	919	rBV	20826975	132509108	100.00%	77.448%
3	14.877	1542	1565	1580	rVV	2021923	8443355	6.37%	4.935%
4	17.777	2168	2188	2228	rBV2	1014701	6108890	4.61%	3.570%
5	33.489	5541	5563	5597	rBV	5424423	19294170	14.56%	11.277%

Sum of corrected areas: 171095053

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Misc : 1 uL PA--Day8 at 1 mL  
ALS Vial : 92 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L  
TIC Integration Parameters: rteint.p



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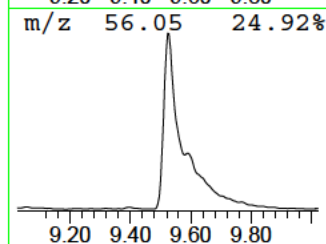
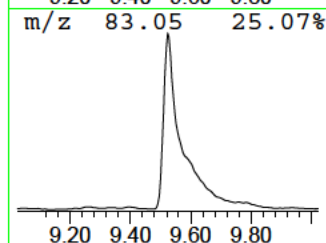
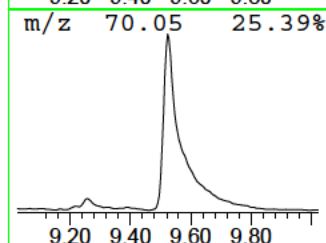
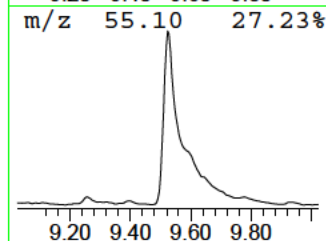
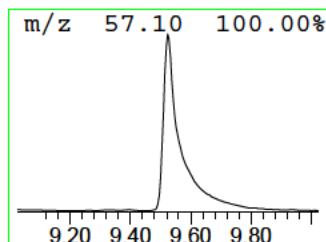
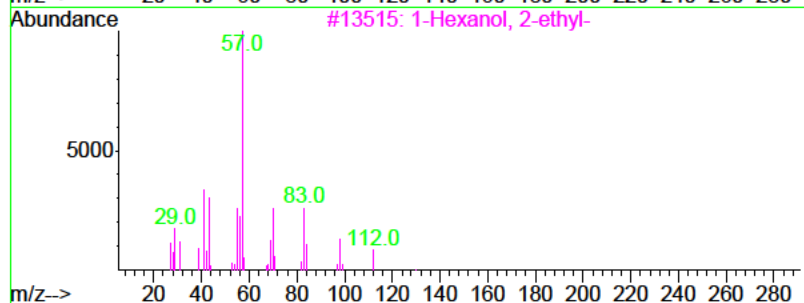
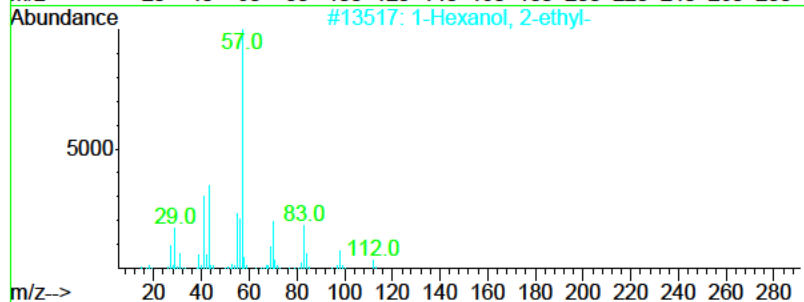
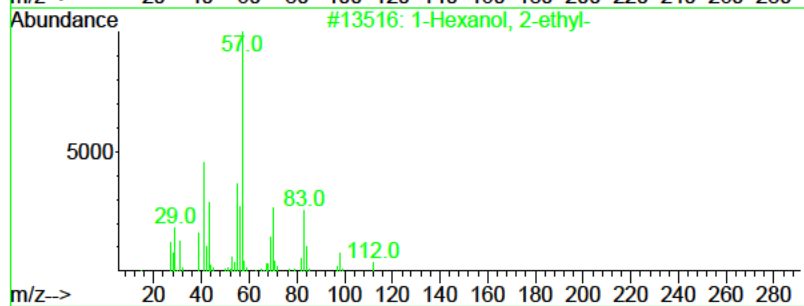
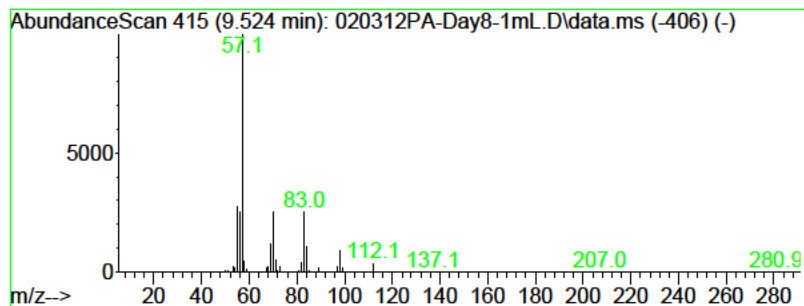
Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L  
TIC Integration Parameters: rteint.p

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Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.524	473.95 ng	4739530	External Standard	0.000

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	59



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Misc : 1 uL PA--Day8 at 1 mL  
ALS Vial : 92 Sample Multiplier: 1

Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

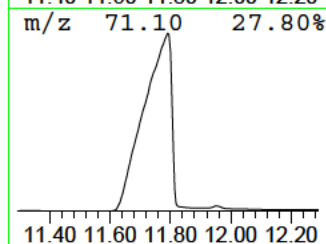
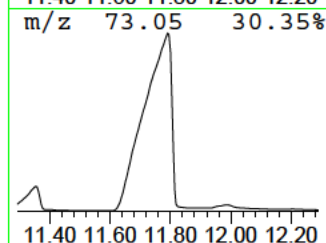
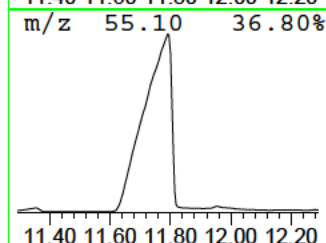
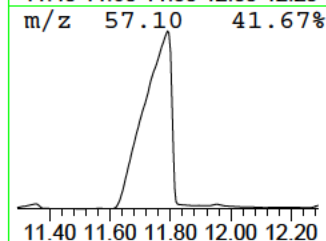
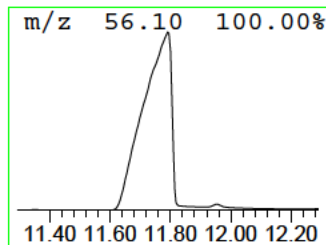
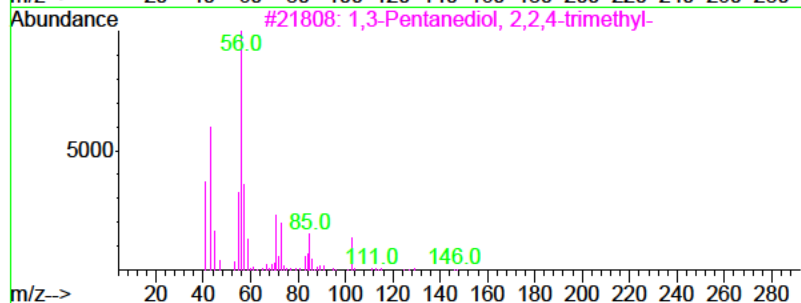
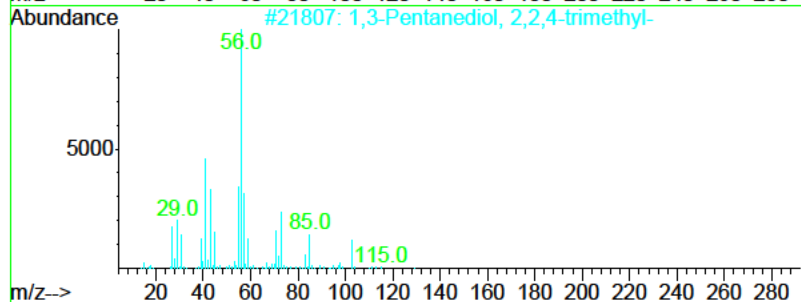
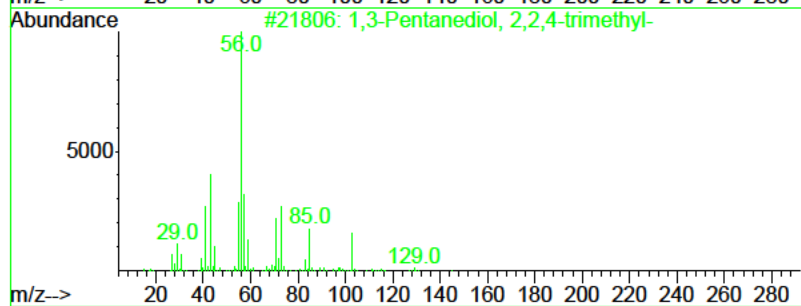
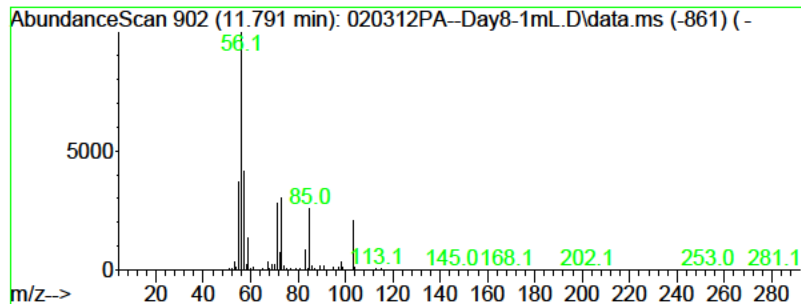
TIC Library : C:\Database\NIST08.L  
TIC Integration Parameters: rteint.p

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Peak Number 2 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.791	13250.90 ng	132509000	External Standard	0.000

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	90
2		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	78
3		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	50
4		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	25
5		Decane, 5-methyl-6-methylene-	168	C12H24	075029-95-7	23



Data Path : C:\msdchem\1\LEGACY\2012\February\  
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Acq On : 3 Feb 2012 8:54  
Operator :  
Sample : PA--Day8-1mL  
Misc : 1 uL PA-B-Day8 at 1 mL  
ALS Vial : 92 Sample Multiplier: 1

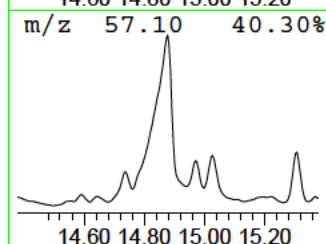
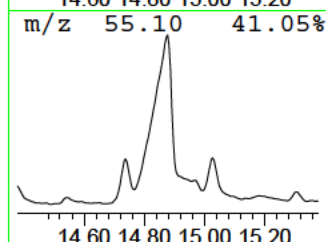
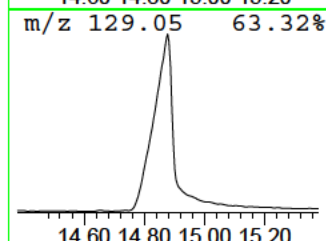
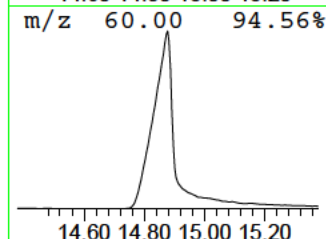
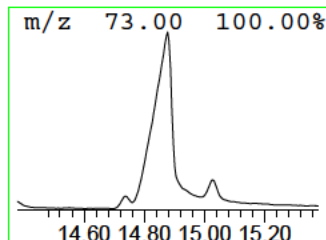
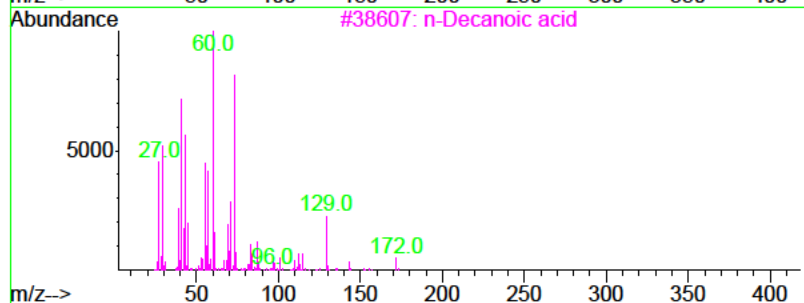
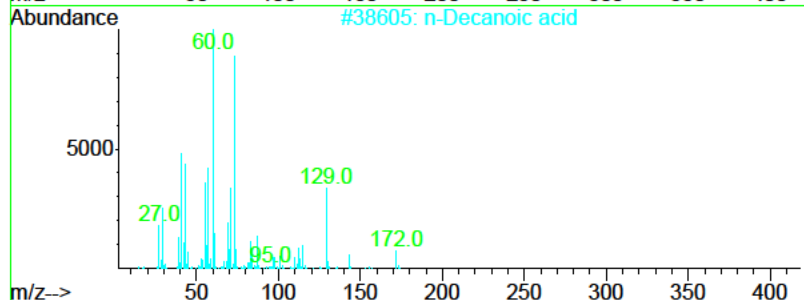
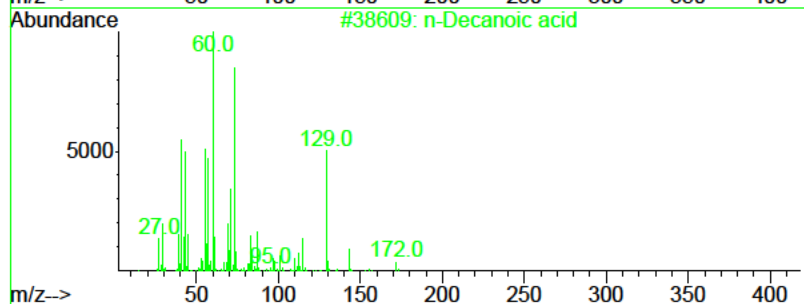
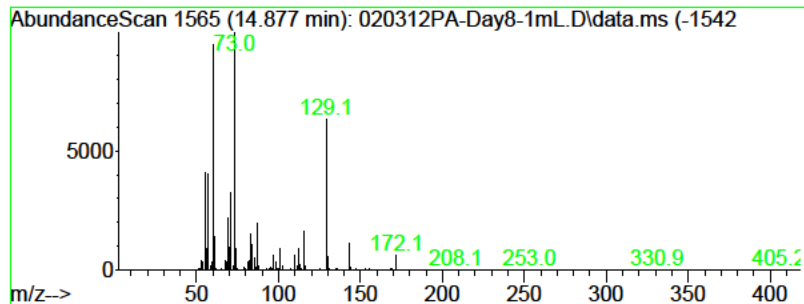
Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L  
TIC Integration Parameters: rteint.p

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Peak Number 3 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.877	844.34 ng	8443360	External Standard	0.000

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	97
2			n-Decanoic acid	172	C10H20O2	000334-48-5	87
3			n-Decanoic acid	172	C10H20O2	000334-48-5	81
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	52



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Sample : PA--Day8-1mL  
Misc : 1 uL PA--Day8 at 1 mL  
ALS Vial : 92 Sample Multiplier: 1

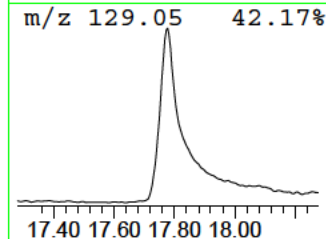
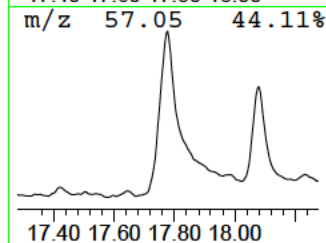
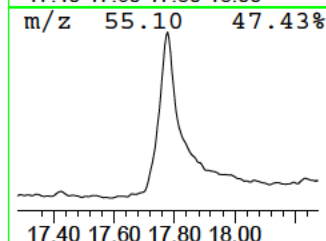
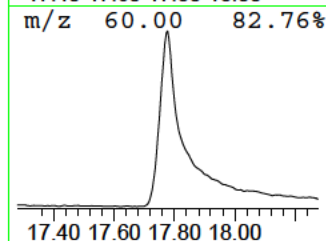
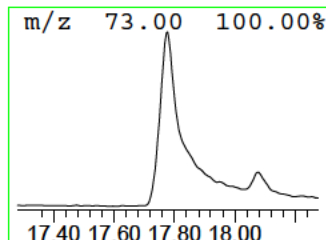
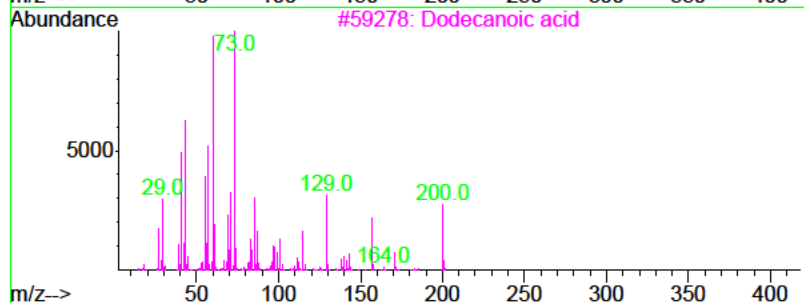
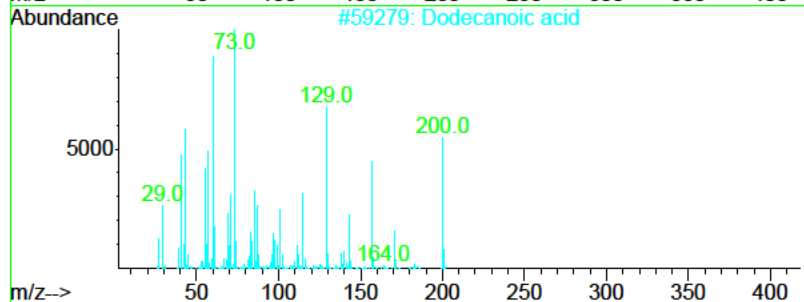
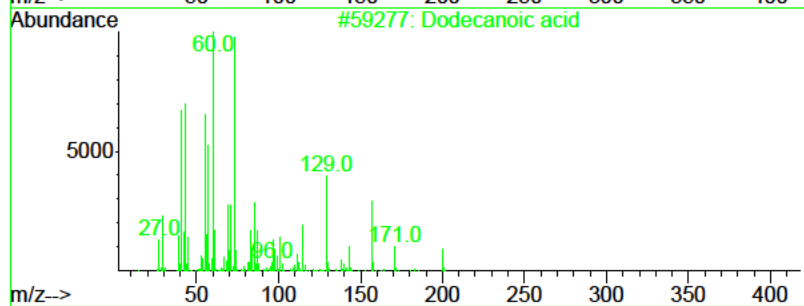
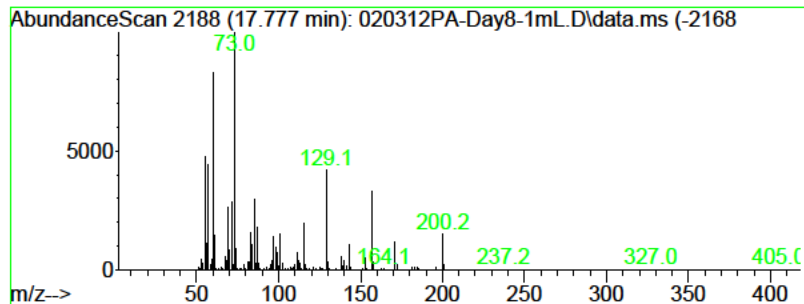
Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L  
TIC Integration Parameters: rteint.p

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Peak Number 4 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.777	610.89 ng	6108890	External Standard	0.000

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	99
2			Dodecanoic acid	200	C12H24O2	000143-07-7	98
3			Dodecanoic acid	200	C12H24O2	000143-07-7	93
4			Dodecanoic acid	200	C12H24O2	000143-07-7	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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Operator :  
Sample : PA- 8-Day8-1mL  
Misc : 1 uL PA--Day8 at 1 mL  
ALS Vial : 92 Sample Multiplier: 1

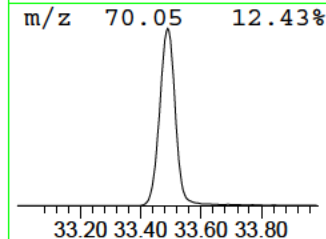
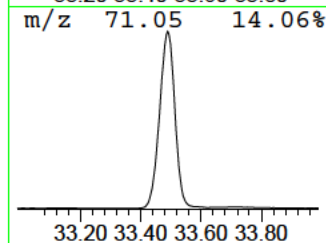
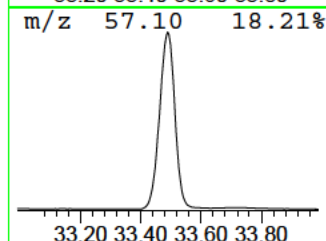
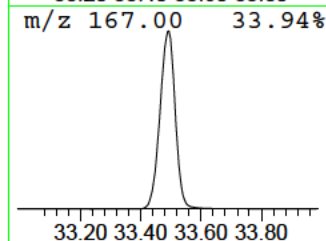
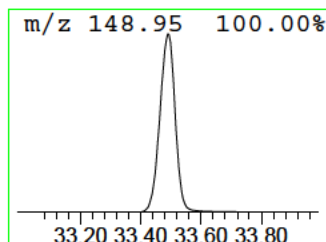
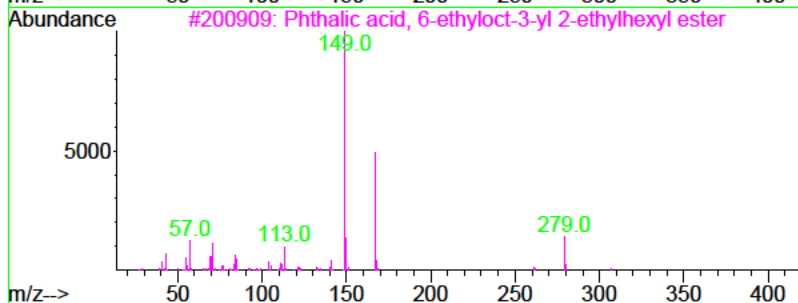
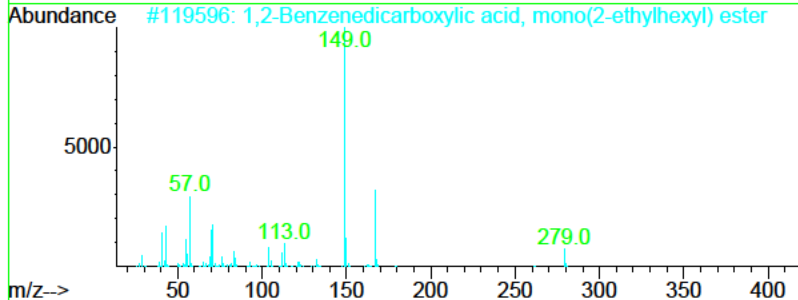
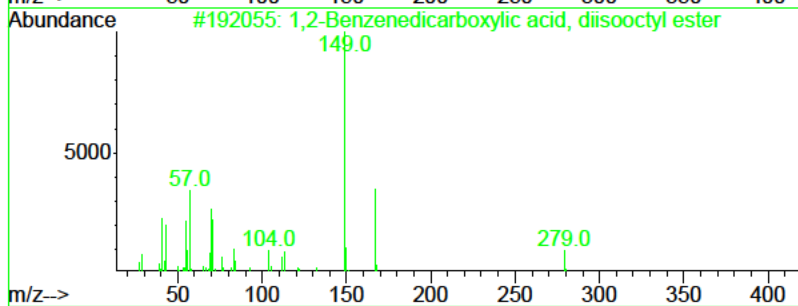
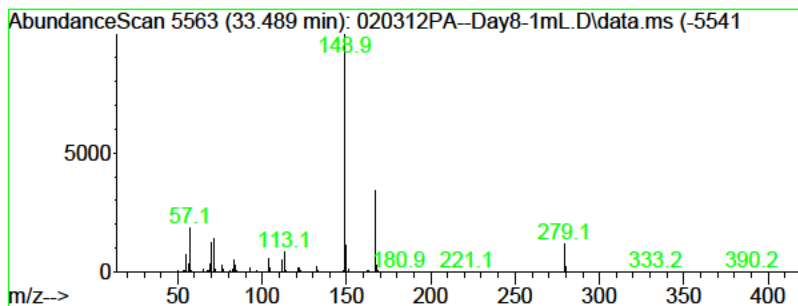
Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L  
TIC Integration Parameters: rteint.p

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Peak Number 5 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
33.489	1929.42 ng	19294200	External Standard	0.000

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	91
2		1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	91
3		Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	86
4		1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	76
5		Phthalic acid, neopentyl 2-penty...	306	C18H26O4	1000315-54-0	59



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Quant Title : PAH5437

TIC Library : C:\Database\NIST08.L  
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard---			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	9.524	474.0	ng	4739530	0	0.000	10000	1.0
1,3-Pentanediol...	11.791	13250.9	ng	132509000	0	0.000	10000	1.0
n-Decanoic acid	14.877	844.3	ng	8443360	0	0.000	10000	1.0
Dodecanoic acid	17.777	610.9	ng	6108890	0	0.000	10000	1.0
1,2-Benzenedica...	33.489	1929.4	ng	19294200	0	0.000	10000	1.0