

Data Path : C:\msdchem\1\LEGACY\2012\February\  
Data File : 020112PA-[REDACTED]-Day6-rerun.D  
Acq On : 1 Feb 2012 11:44  
Operator :  
Sample : PA-[REDACTED]-Day6-rerun  
Misc : 1 uL PA-[REDACTED]-Day6-rerun at 1 mL  
ALS Vial : 85 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: 020112PA-[REDACTED]-Day6-rerun.D\data.ms

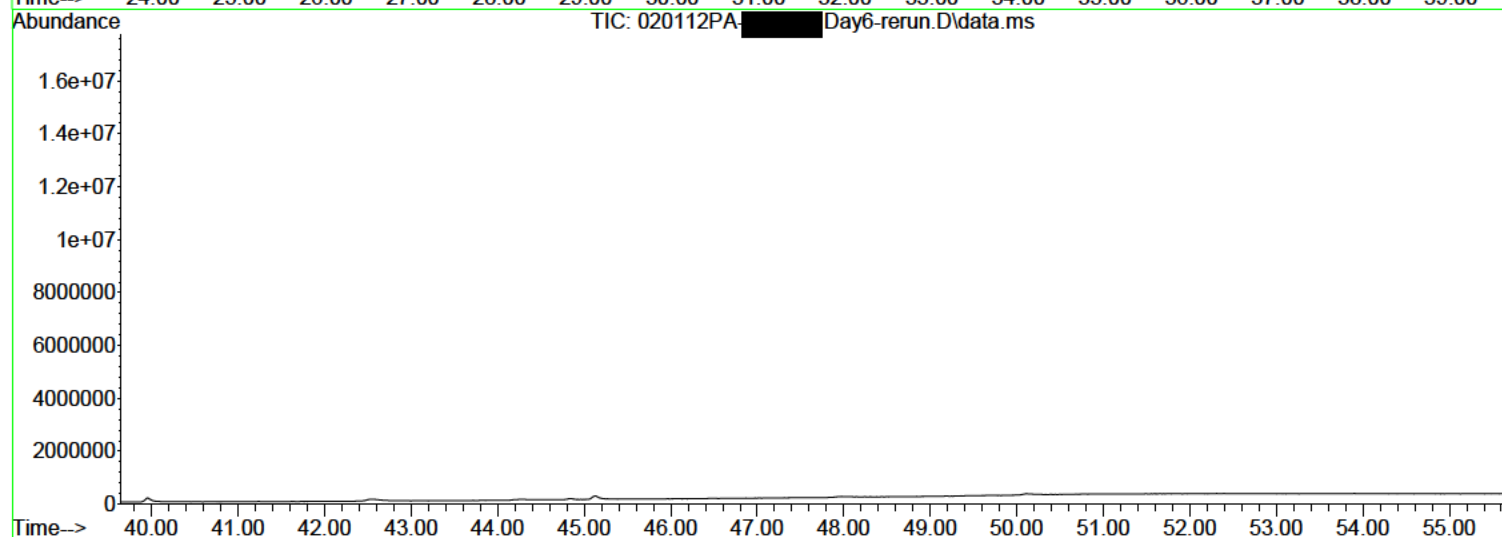
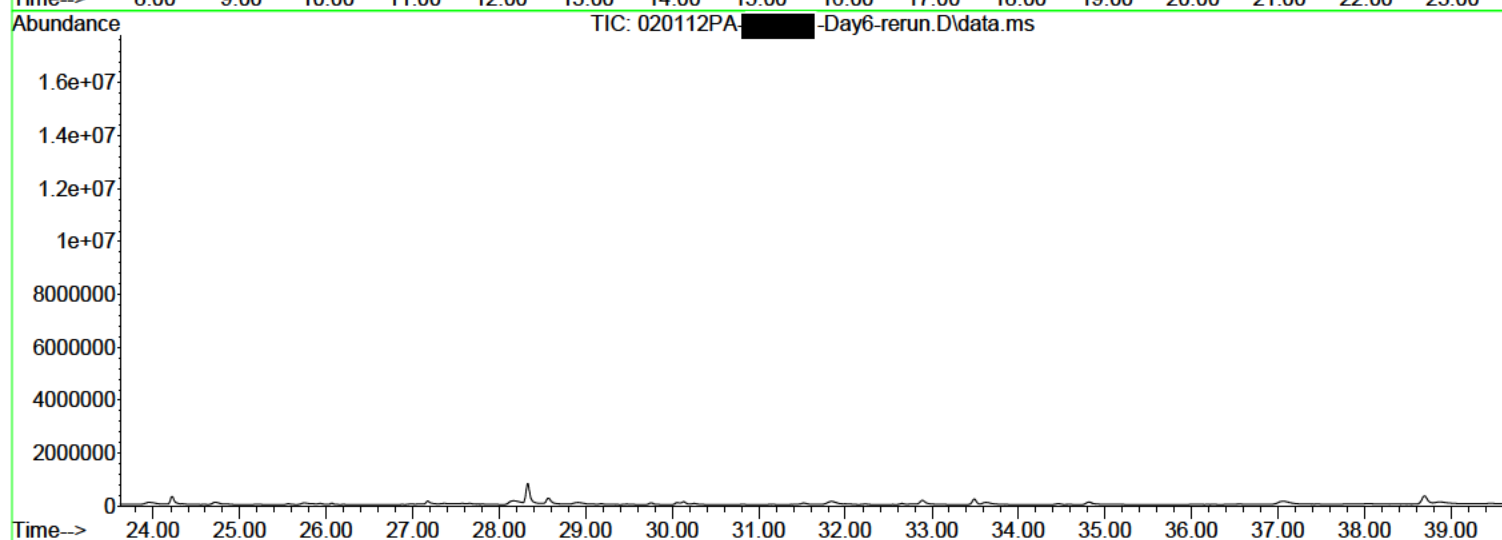
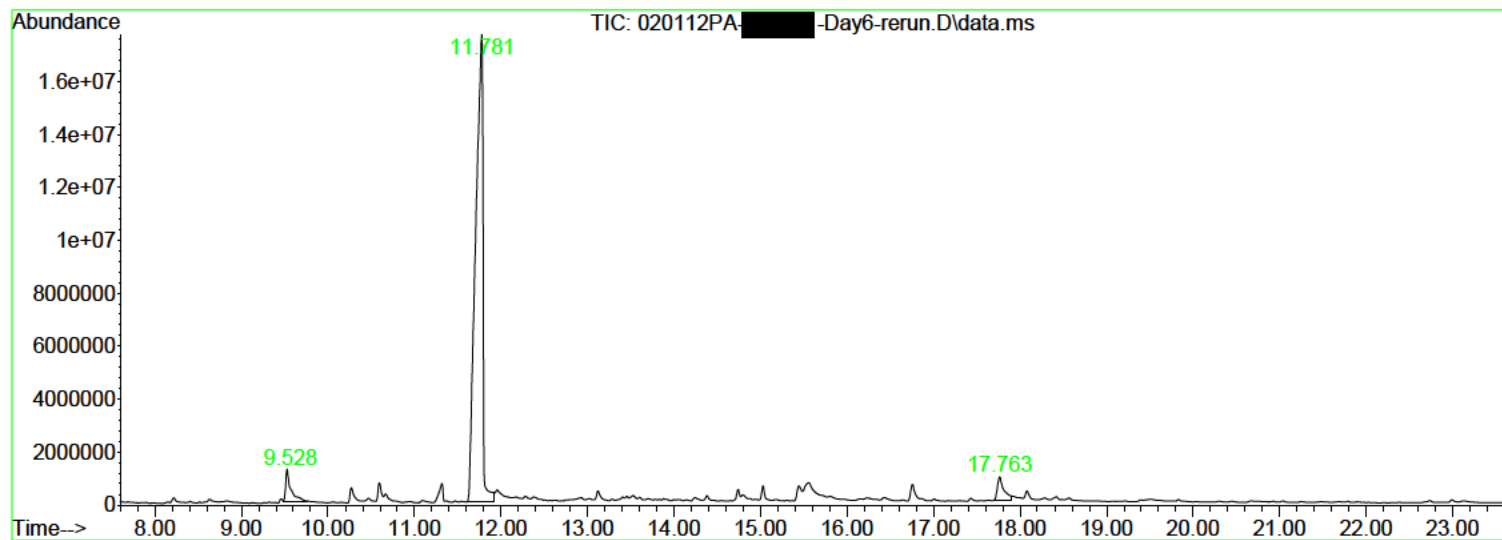
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.528	407	416	465	rVB2	1203557	4806970	4.61%	4.221%
2	11.781	862	900	931	rBV	17674314	104339827	100.00%	91.626%
3	17.763	2171	2185	2216	rBV2	882264	4728616	4.53%	4.152%

Sum of corrected areas: 113875413

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ALS Vial : 85 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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Misc : 1 uL PA-[REDACTED]-Day6-rerun at 1 mL  
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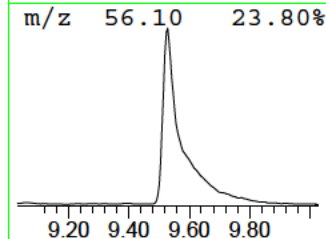
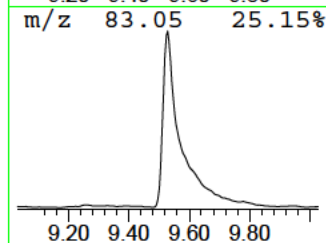
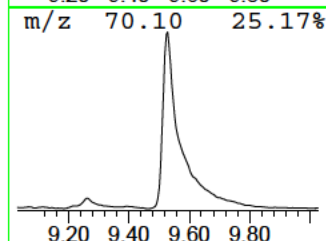
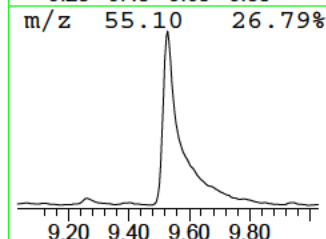
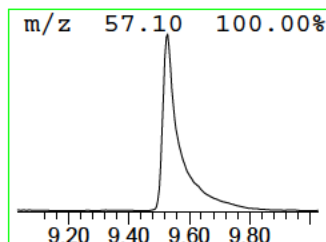
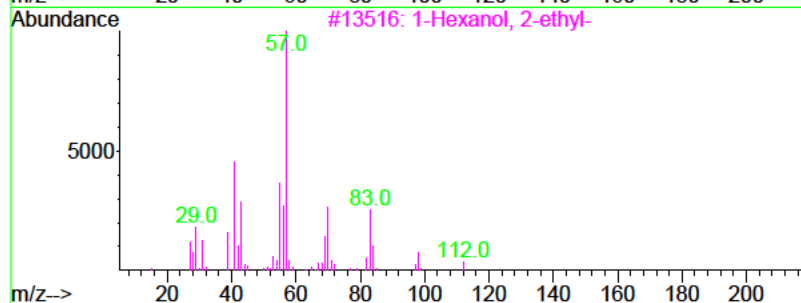
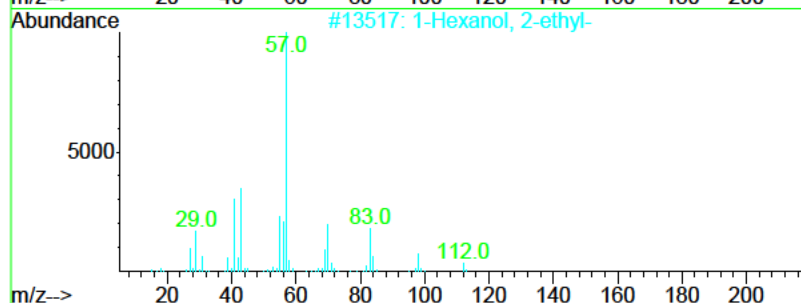
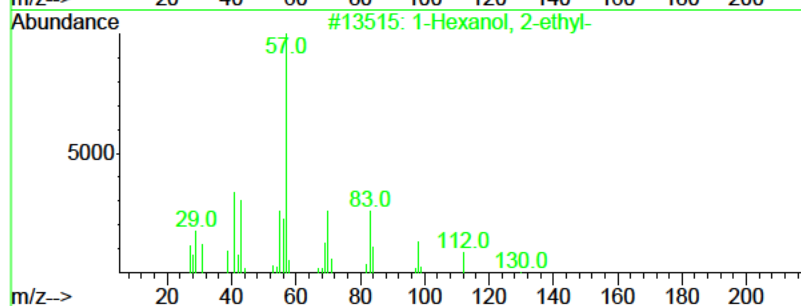
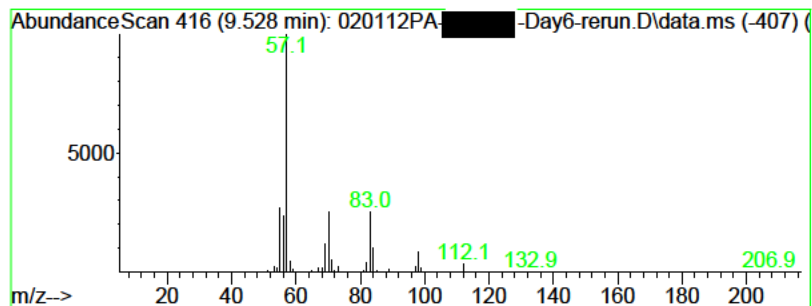
Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.528	480.70 ng	4806970	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	64
5			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	59



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ALS Vial : 85 Sample Multiplier: 1

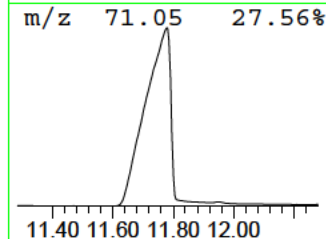
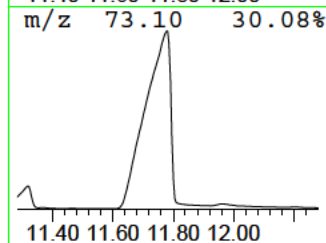
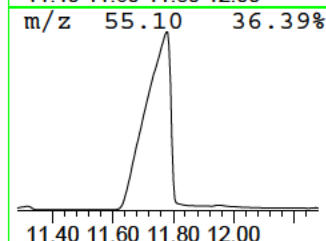
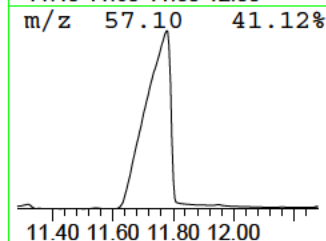
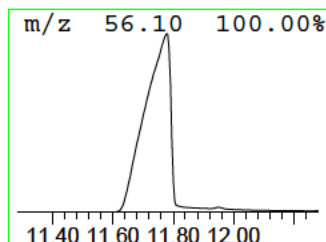
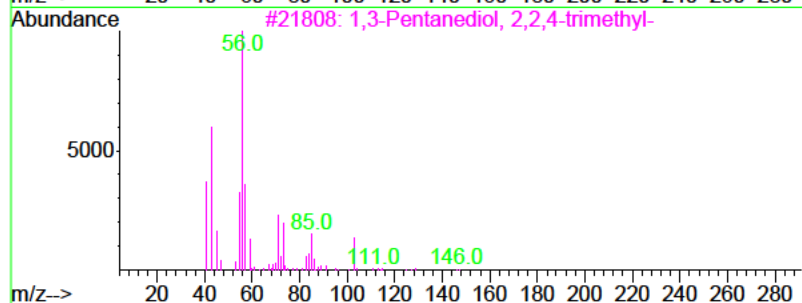
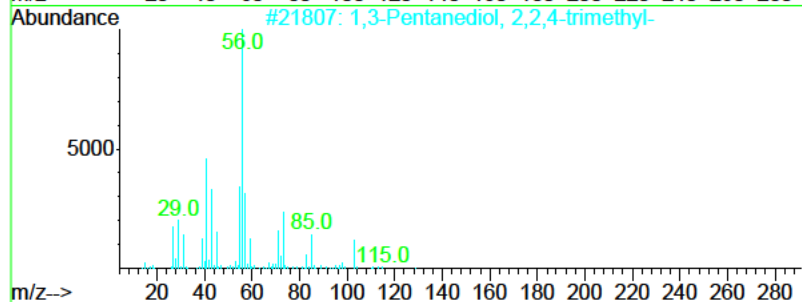
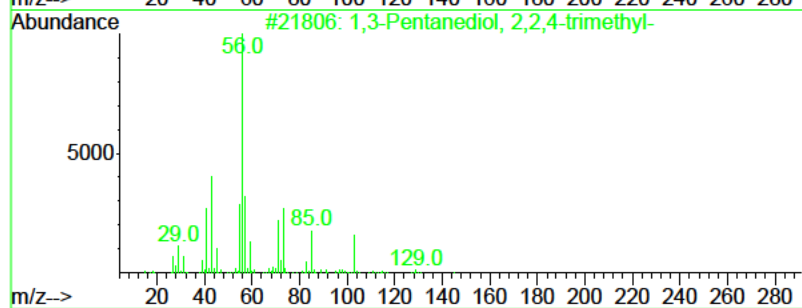
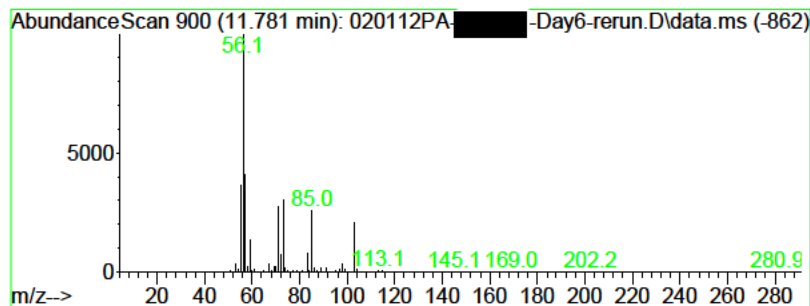
Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

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

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Peak Number 2 1,3-Pentanediol, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.781	10434.00 ng	104340000	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	53
4		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	25
5		Decane, 5-methyl-6-methylene-	168	C12H24	075029-95-7	23



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Misc : 1 uL PA- -Day6-rerun at 1 mL  
ALS Vial : 85 Sample Multiplier: 1

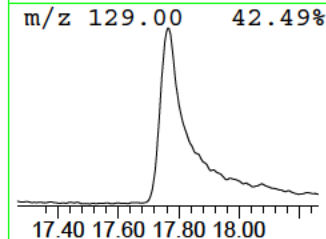
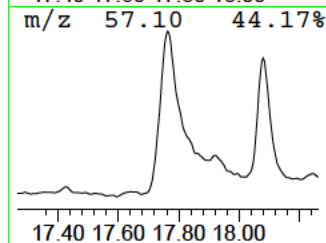
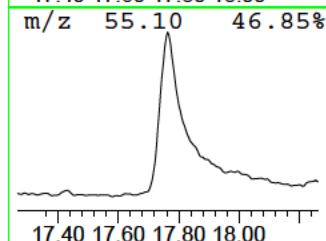
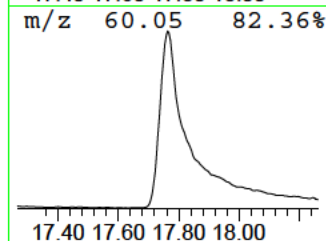
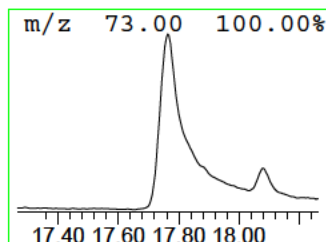
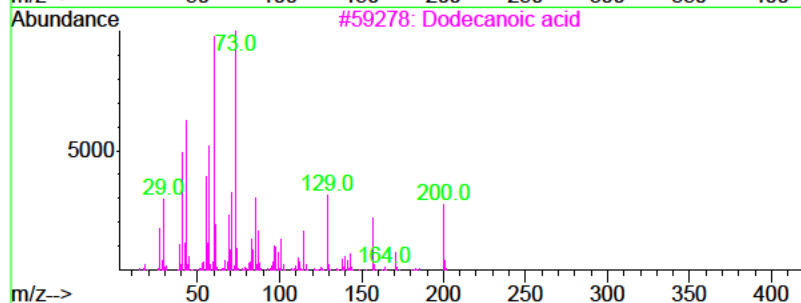
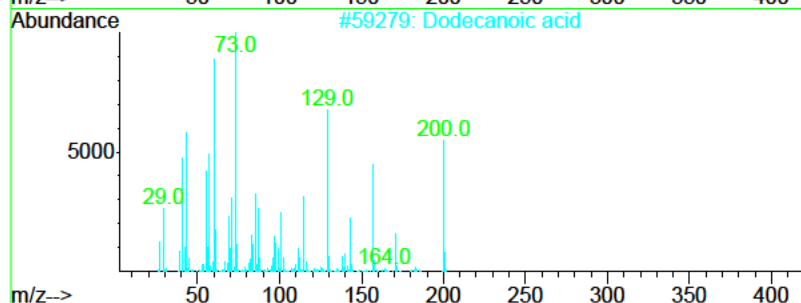
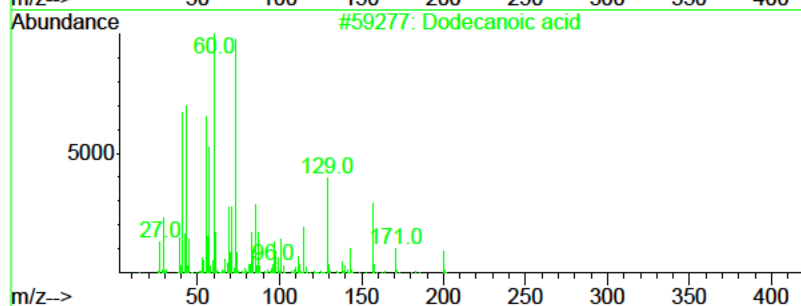
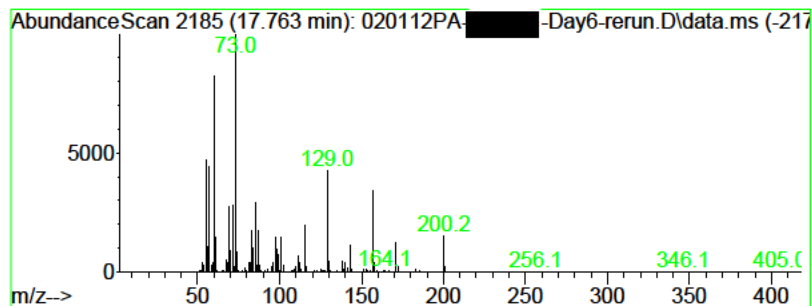
Quant Method : C:\msdchem\1\METHODS\TLTICPAH.M  
Quant Title : PAH5437

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

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Peak Number 3 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.763	472.86 ng	4728620	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	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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Misc : 1 uL PA-[REDACTED]-Day6-rerun at 1 mL  
ALS Vial : 85 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard---			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	9.528	480.7	ng	4806970	0	0.000	10000	1.0
1,3-Pentenediol...	11.781	10434.0	ng	104340000	0	0.000	10000	1.0
Dodecanoic acid	17.763	472.9	ng	4728620	0	0.000	10000	1.0