

Data Path : Z:\HPCHEM1\BNA G\Data\BG032517\
 Data File : BG026423.D
 Acq On : 24 Mar 2017 20:29
 Operator : SJ/MA
 Sample : I2378-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 53A-9-11

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032017.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.143	344	350	359	rBV	235425	359424	3.34%	0.653%
2	5.619	424	431	449	rBV	2461224	3904469	36.32%	7.090%
3	7.211	693	702	714	rBV	2239846	3875152	36.05%	7.037%
4	7.582	757	765	772	rBV	2456153	4281164	39.83%	7.774%
5	8.046	837	844	851	rVB	433798	732107	6.81%	1.329%
6	8.369	889	899	911	rVB	1990002	3454812	32.14%	6.274%
7	9.203	1032	1041	1051	rBV	1392067	2457921	22.87%	4.463%
8	10.842	1311	1320	1332	rBV	588990	1076918	10.02%	1.956%
9	13.275	1727	1734	1746	rBV	4155258	6830022	63.54%	12.403%
10	14.097	1867	1874	1885	rBV	807599	1222164	11.37%	2.219%
11	14.650	1961	1968	1979	rBV2	946918	1495837	13.92%	2.716%
12	16.130	2212	2220	2239	rBV	3318393	5115557	47.59%	9.290%
13	17.382	2426	2433	2445	rBV	1256994	1945967	18.10%	3.534%
14	18.040	2540	2545	2550	rVB	88024	112624	1.05%	0.205%
15	18.257	2577	2582	2590	rBV	415729	620664	5.77%	1.127%
16	18.328	2591	2594	2599	rVB	77925	109744	1.02%	0.199%
17	19.115	2723	2728	2737	rBV3	142188	279730	2.60%	0.508%
18	19.520	2793	2797	2805	rBV2	163981	257263	2.39%	0.467%
19	19.979	2869	2875	2885	rBV	8032277	10748853	100.00%	19.519%
20	21.271	3090	3095	3104	rBV	243158	473708	4.41%	0.860%
21	21.506	3131	3135	3140	rVB	99957	136845	1.27%	0.249%
22	21.624	3149	3155	3169	rBV	1630611	2638862	24.55%	4.792%
23	22.464	3293	3298	3309	rVB6	53113	120415	1.12%	0.219%
24	22.776	3346	3351	3357	rVB2	100787	168753	1.57%	0.306%
25	24.803	3686	3696	3711	rVB2	948755	2649128	24.65%	4.811%

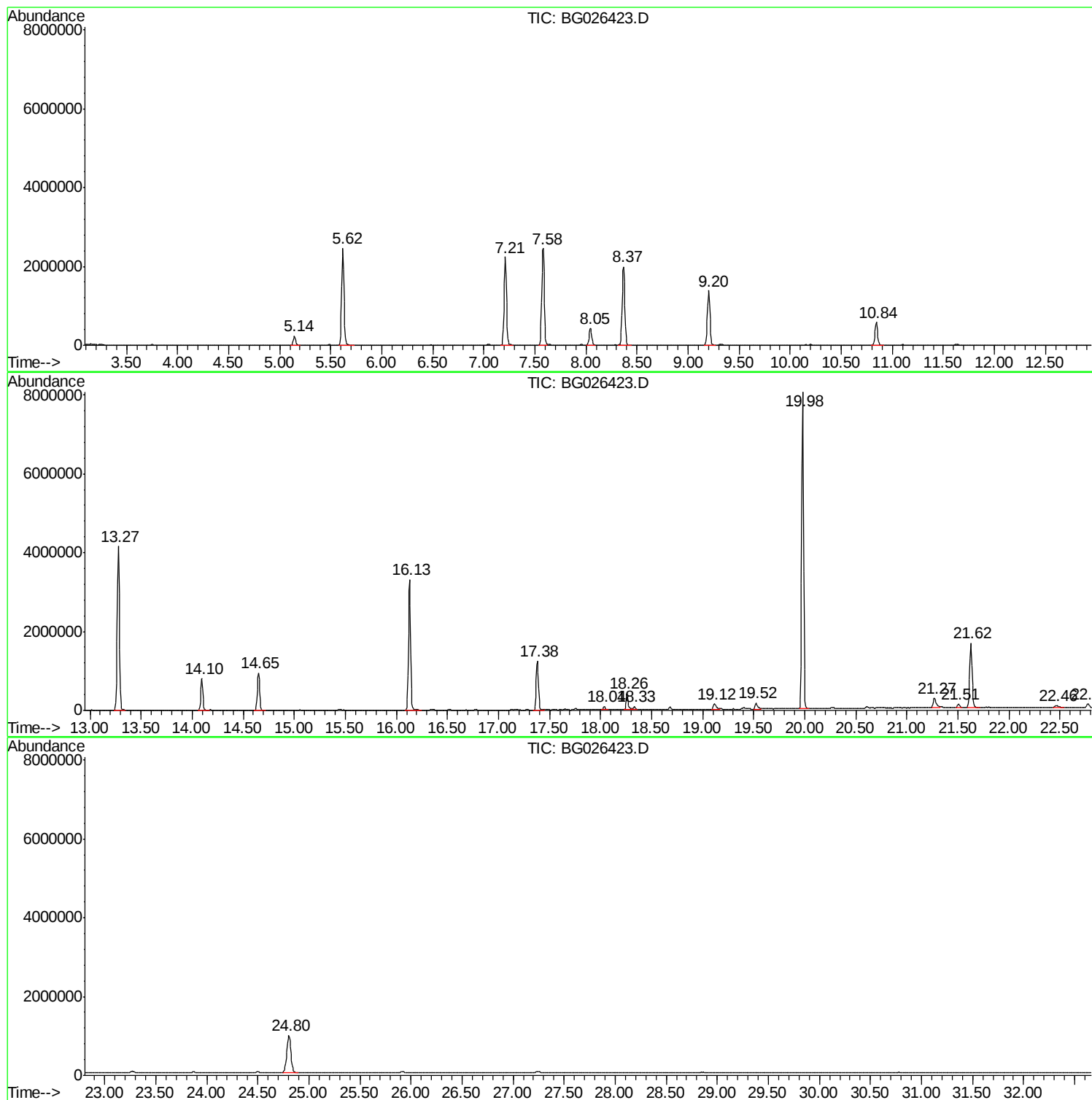
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Operator : SJ/MA
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampled :
53A-9-11

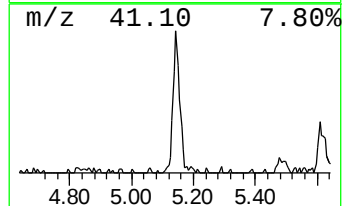
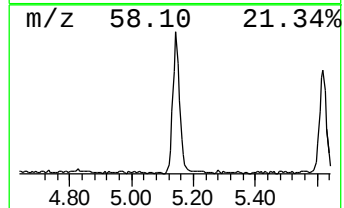
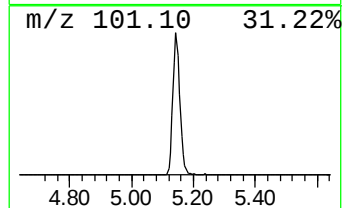
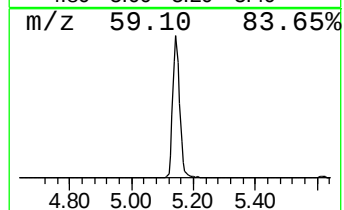
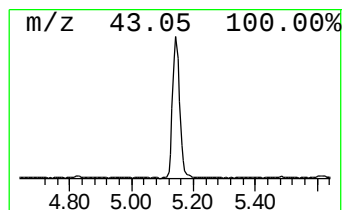
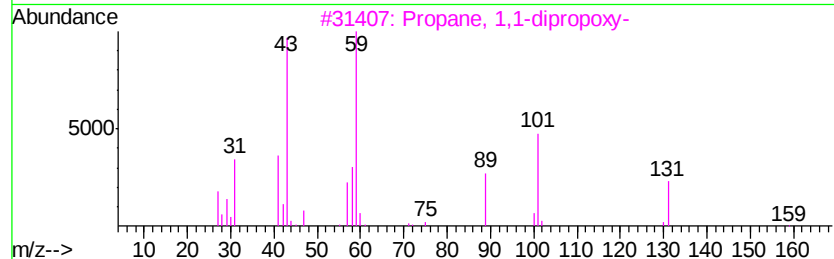
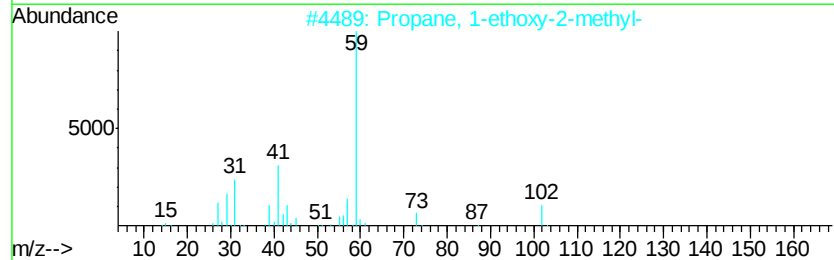
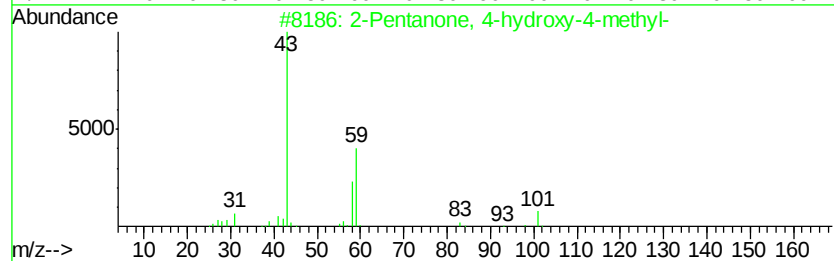
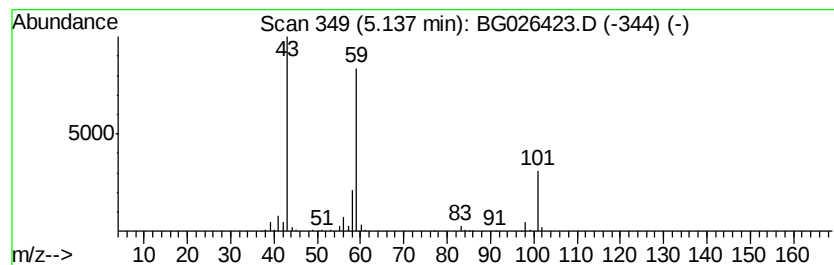
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	9.82 ng	359424	1,4-Dichlorobenzene-d4	8.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43
3			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	40
4			(2,3,3-Trimethyloxiran-1-yl)methanol	116	C6H12O2	1000306-64-7	39
5			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33



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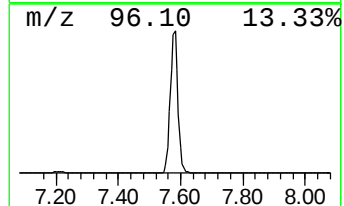
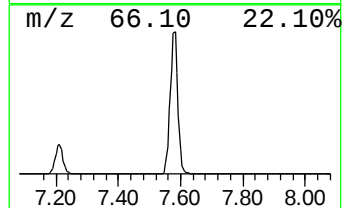
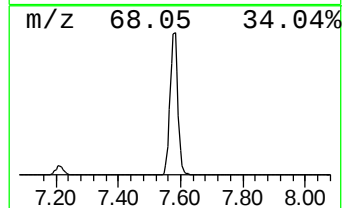
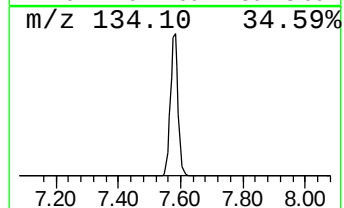
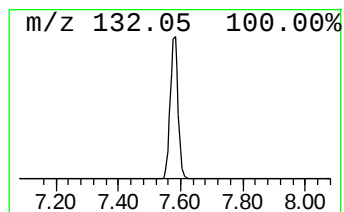
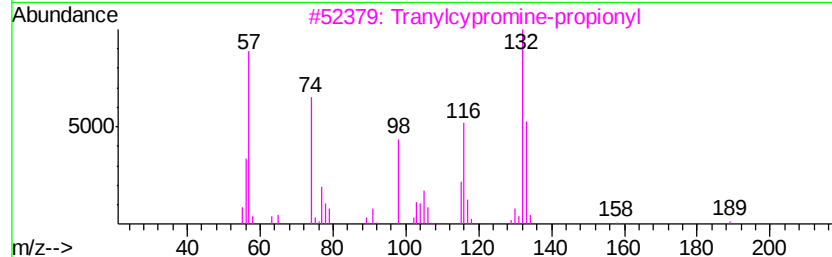
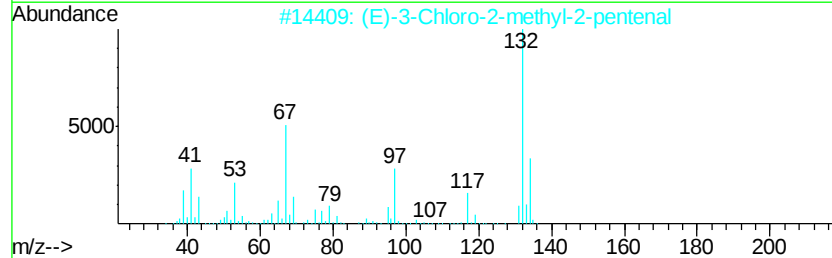
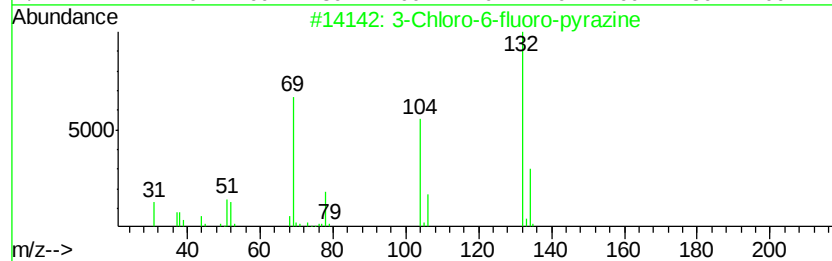
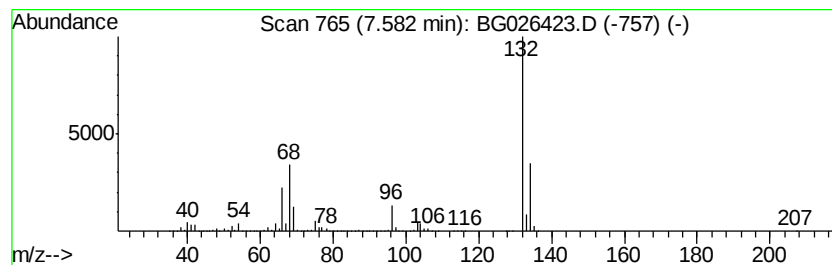
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	116.96 ng	4281160	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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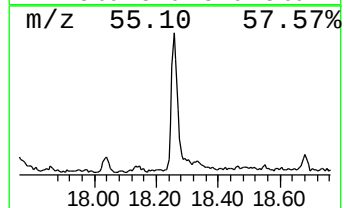
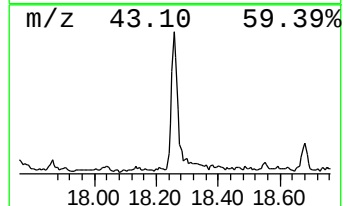
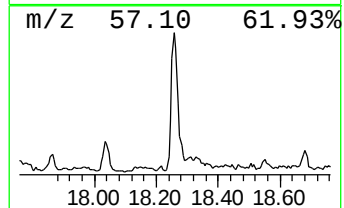
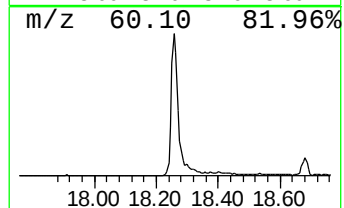
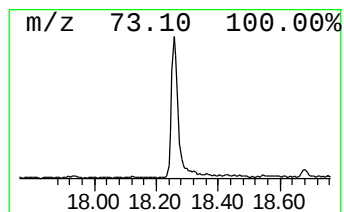
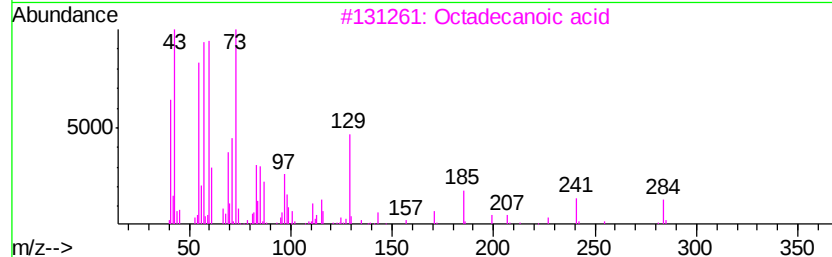
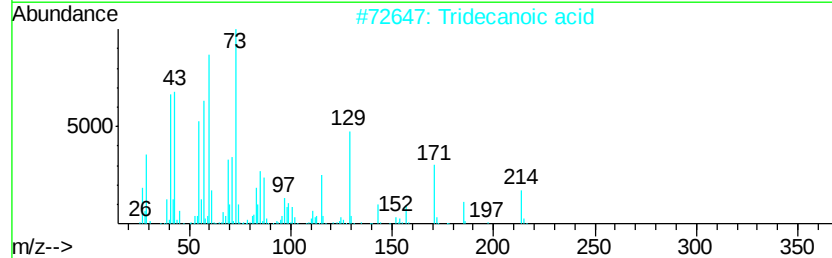
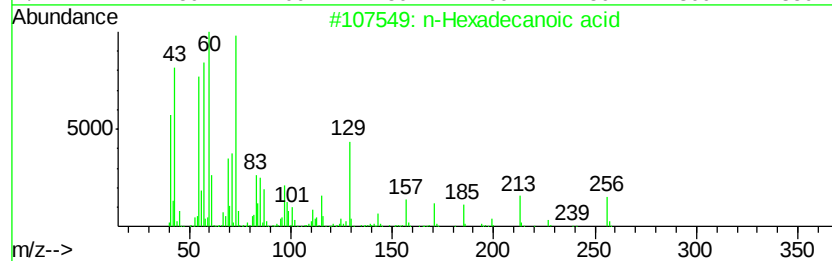
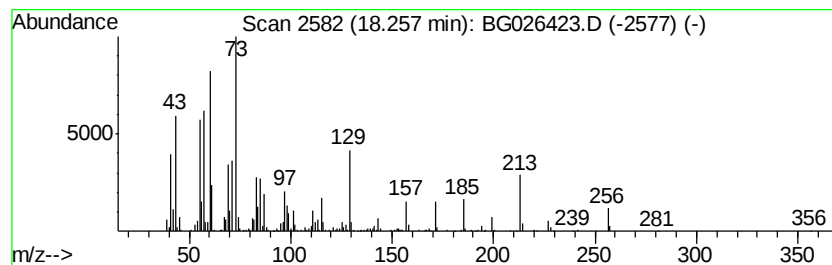
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.26	6.38 ng	620664	Phenanthrene-d10		17.38	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	95
3	Octadecanoic acid		284	C18H36O2	000057-11-4	81
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	74
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	72



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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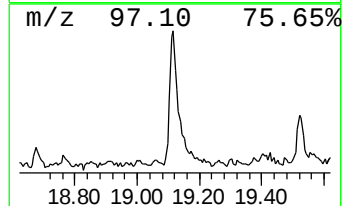
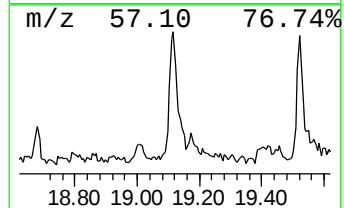
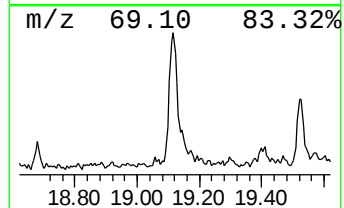
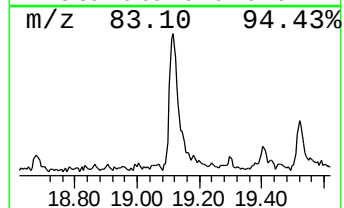
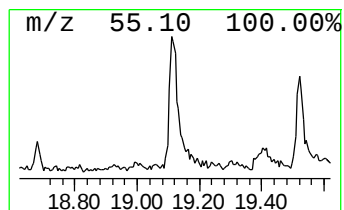
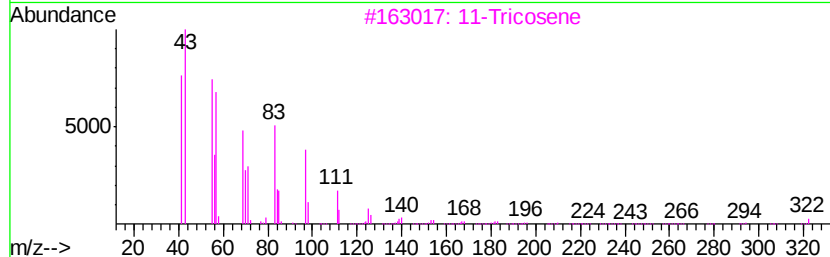
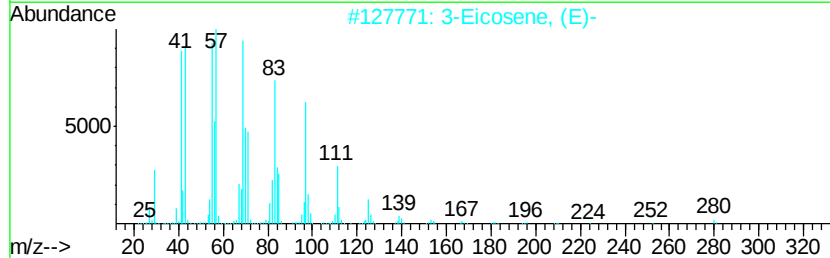
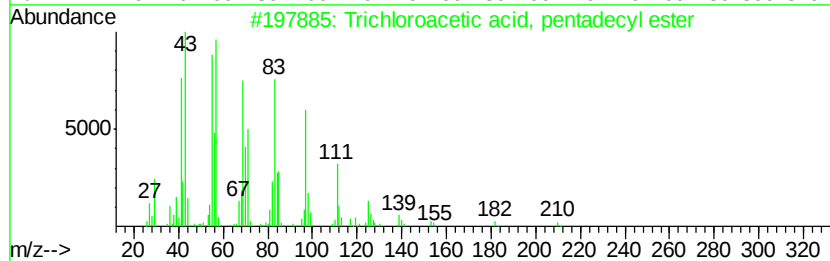
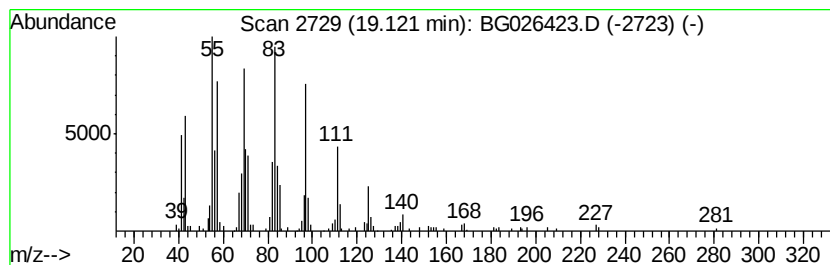
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Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	2.87 ng	279730	Phenanthrene-d10	17.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		11-Tricosene	322	C23H46	052078-56-5	91
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



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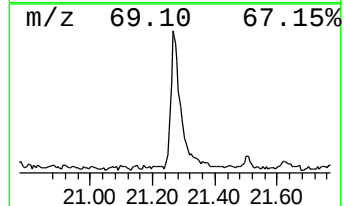
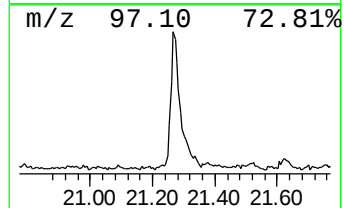
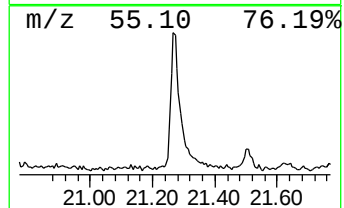
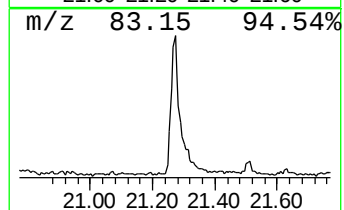
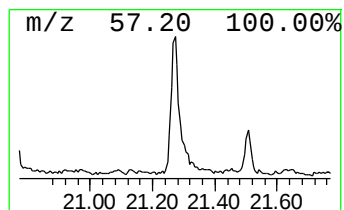
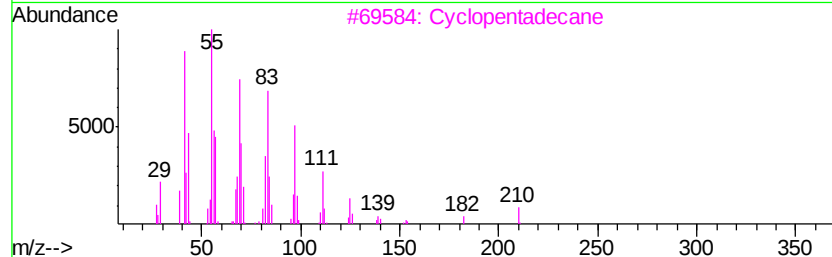
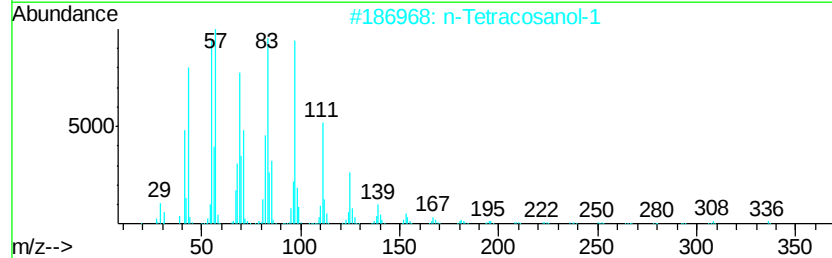
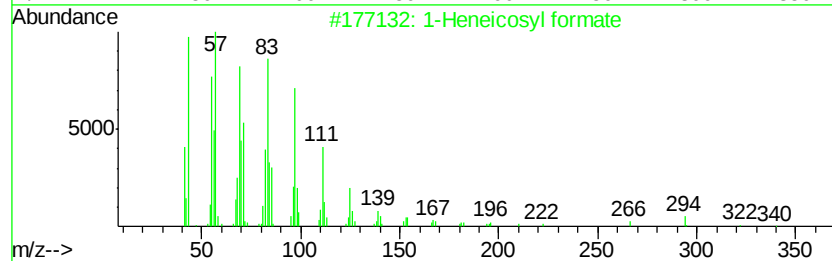
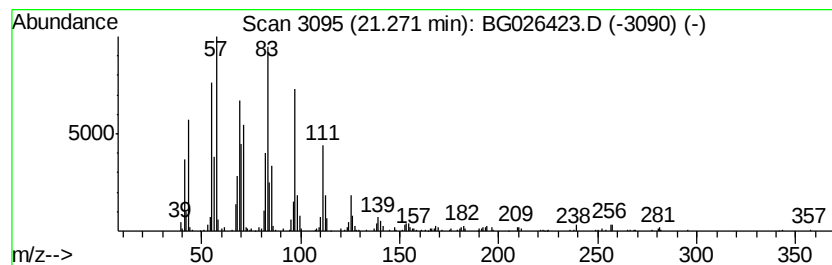
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Peak Number 6 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
21.27	3.59 ng	473708	Chrysene-d12		21.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3			Cyclopentadecane	210	C15H30	000295-48-7	93
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	9.8	ng	359424	1	8.04	732107	20.0
unknown7.58	7.58	117.0	ng	4281160	1	8.04	732107	20.0
n-Hexadecanoic acid	18.26	6.4	ng	620664	4	17.38	1945970	20.0
Trichloroacetic a...	19.12	2.9	ng	279730	4	17.38	1945970	20.0
1-Heneicosyl formate	21.27	3.6	ng	473708	5	21.62	2638860	20.0