

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031819\
 Data File : BM019218.D
 Acq On : 18 Mar 2019 16:39
 Operator : JU/SJ
 Sample : K1935-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-17(0.5-1.5)

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 : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.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	5.251	378	385	404	rBV	2928913	4448712	48.04%	7.161%
2	6.834	646	654	674	rBV	3331278	5629133	60.79%	9.061%
3	7.187	706	714	730	rBV	3331766	5388873	58.19%	8.674%
4	7.645	786	792	800	rBV	741389	1185557	12.80%	1.908%
5	7.963	839	846	858	rBV	2427532	3821743	41.27%	6.152%
6	8.816	984	991	1010	rBV	1867794	3357431	36.26%	5.404%
7	10.433	1258	1266	1286	rBV	1024638	1823457	19.69%	2.935%
8	12.916	1681	1688	1711	rBV	5244379	7885263	85.15%	12.692%
9	13.774	1828	1834	1847	rBV	304269	511346	5.52%	0.823%
10	14.304	1917	1924	1945	rBV2	1649860	2619326	28.29%	4.216%
11	15.804	2173	2179	2199	rBV	3741094	5514992	59.55%	8.877%
12	17.056	2386	2392	2404	rBV	1933909	2914293	31.47%	4.691%
13	17.951	2538	2544	2553	rBV	231503	396808	4.28%	0.639%
14	19.239	2759	2763	2769	rBV	64685	100883	1.09%	0.162%
15	19.697	2835	2841	2859	rBV	7377580	9260403	100.00%	14.906%
16	20.962	3052	3056	3067	rBV2	315565	535437	5.78%	0.862%
17	21.256	3101	3106	3119	rBV	1904902	2651226	28.63%	4.267%
18	21.392	3126	3129	3133	rBV	113151	123998	1.34%	0.200%
19	21.827	3199	3203	3206	rBV	183453	224973	2.43%	0.362%
20	22.280	3277	3280	3287	rVB	269553	323523	3.49%	0.521%
21	22.780	3361	3365	3370	rBV	289124	415747	4.49%	0.669%
22	23.344	3457	3461	3467	rVB	258750	390132	4.21%	0.628%
23	23.491	3480	3486	3498	rVB2	1104424	2235313	24.14%	3.598%
24	23.985	3566	3570	3576	rVB	219596	367750	3.97%	0.592%

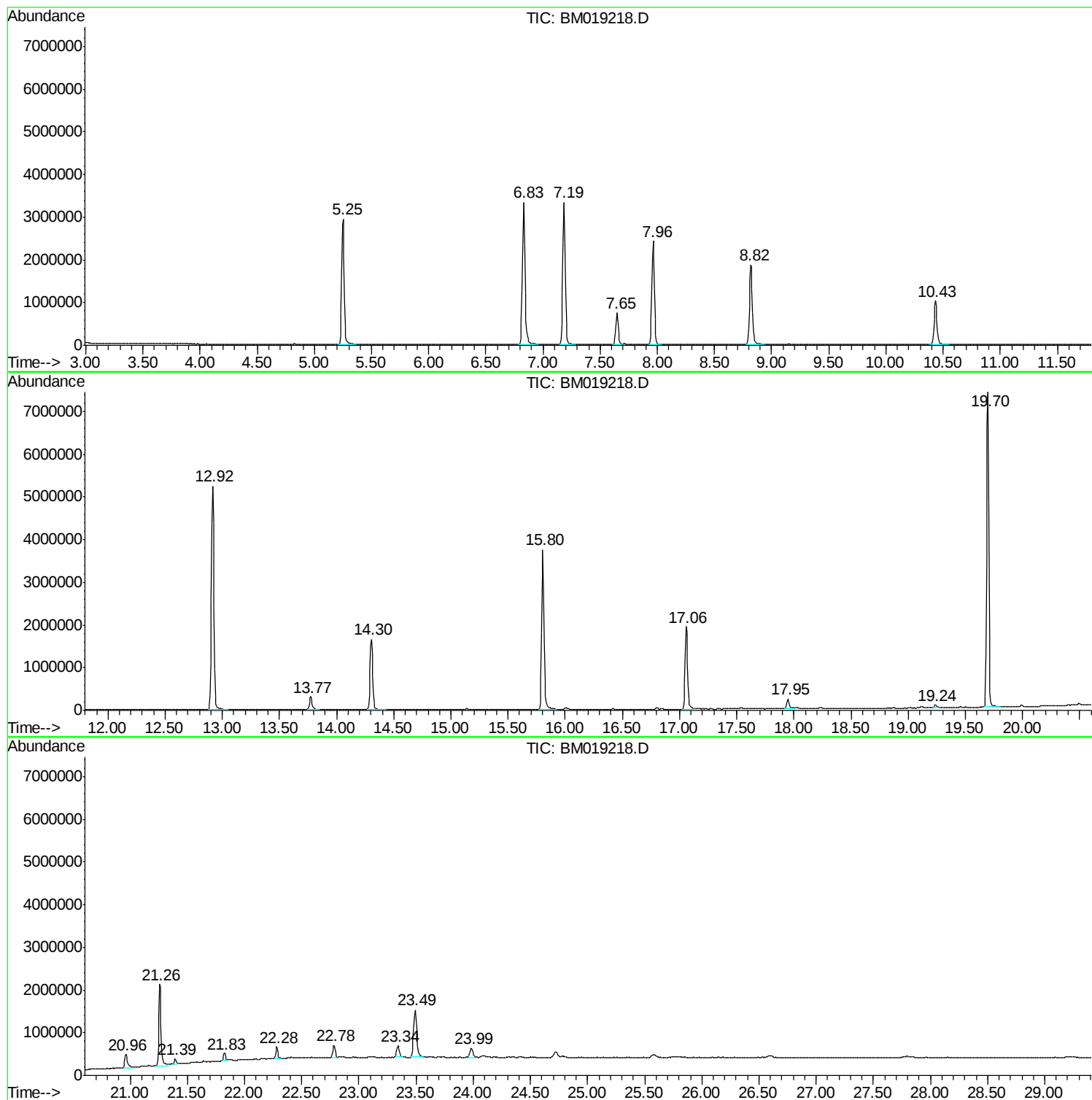
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Acq On : 18 Mar 2019 16:39
Operator : JU/SJ
Sample : K1935-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampled :
SB-17(0.5-1.5)

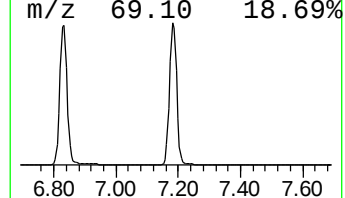
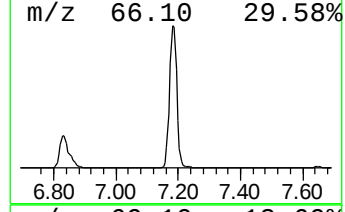
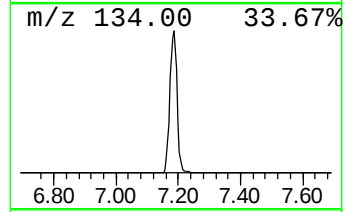
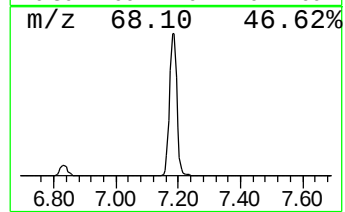
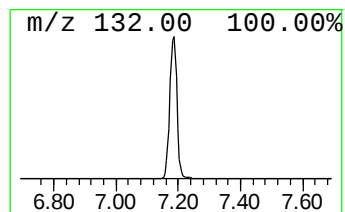
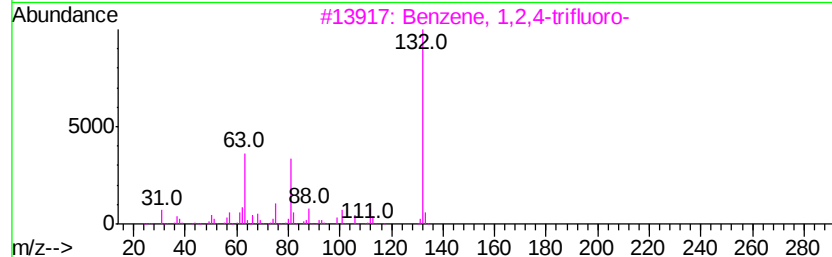
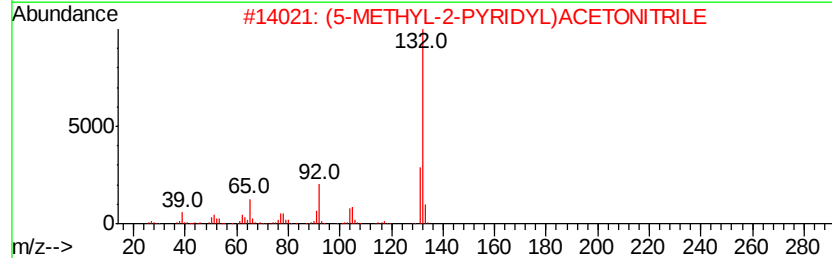
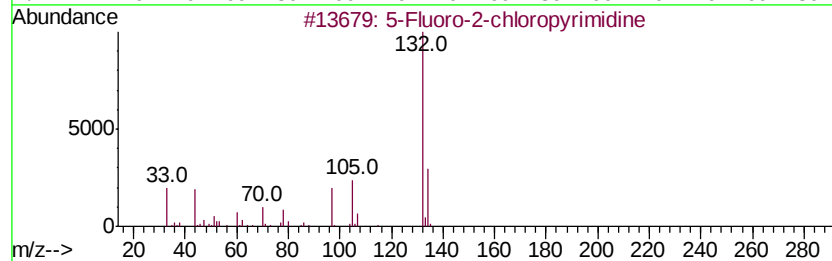
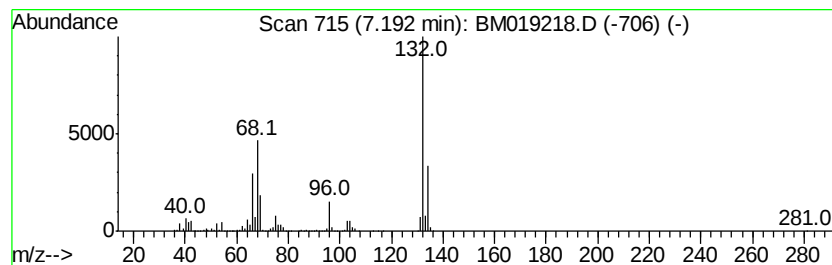
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	90.91 ng	5388870	1,4-Dichlorobenzene-d4	7.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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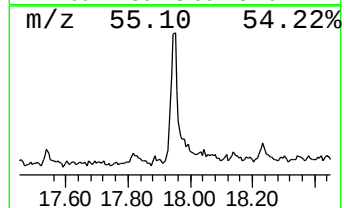
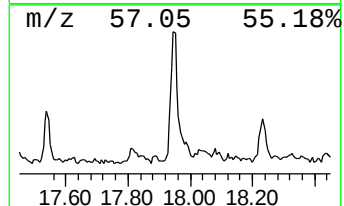
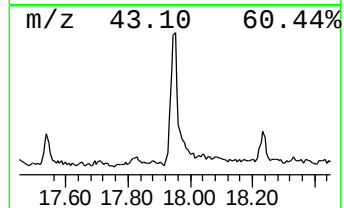
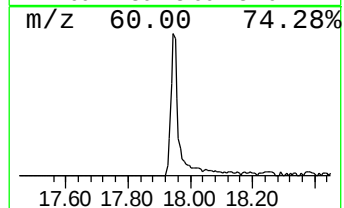
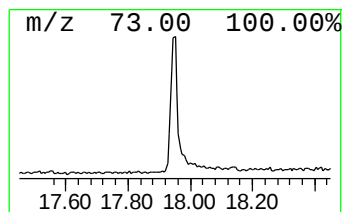
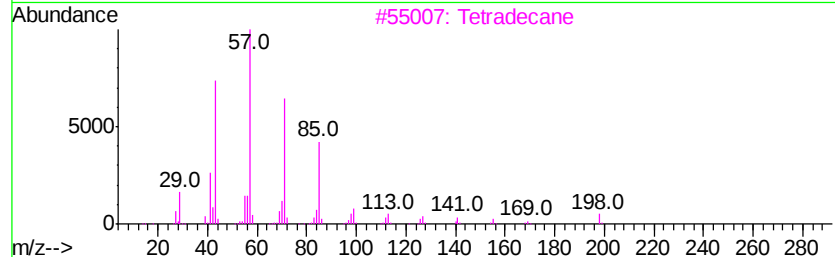
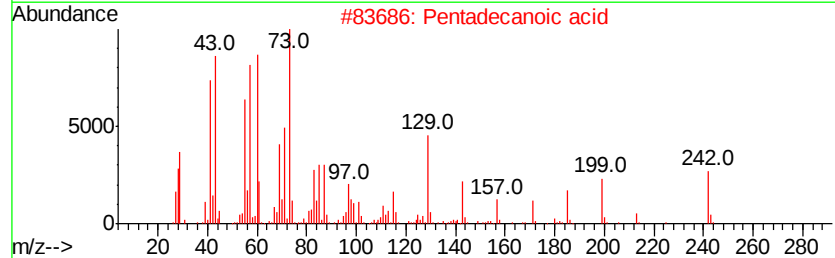
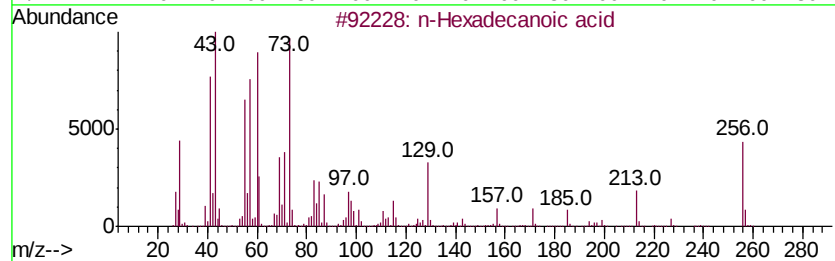
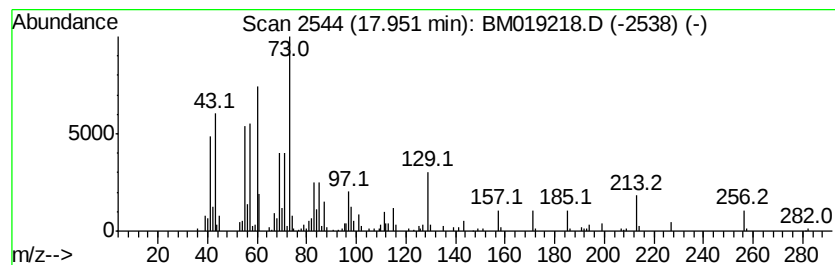
Instrument :
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.95	2.72 ng	396808	Phenanthrene-d10		17.06
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecane	198	C14H30	000629-59-4	11
4	Dodecane	170	C12H26	000112-40-3	11
5	Eicosane	282	C20H42	000112-95-8	11



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Instrument :
BNA_M
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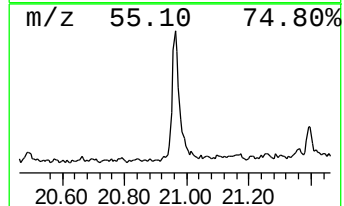
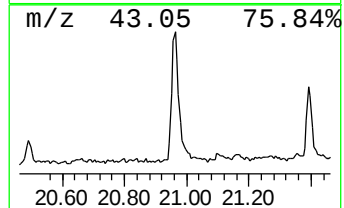
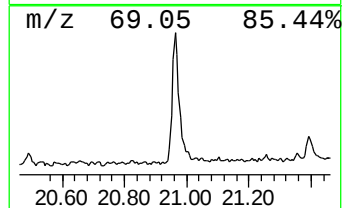
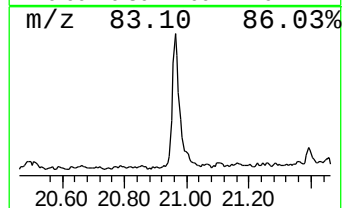
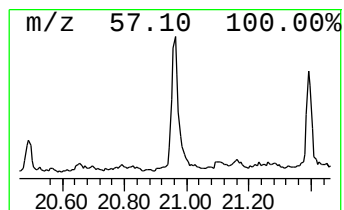
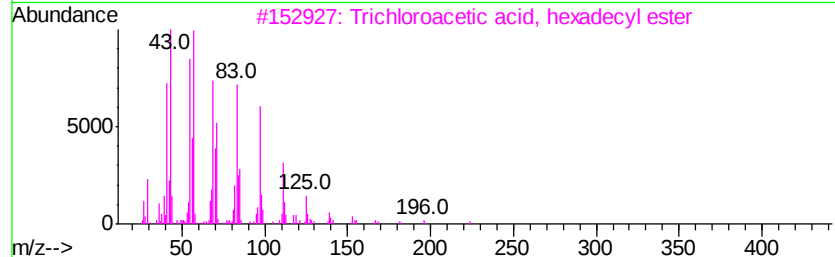
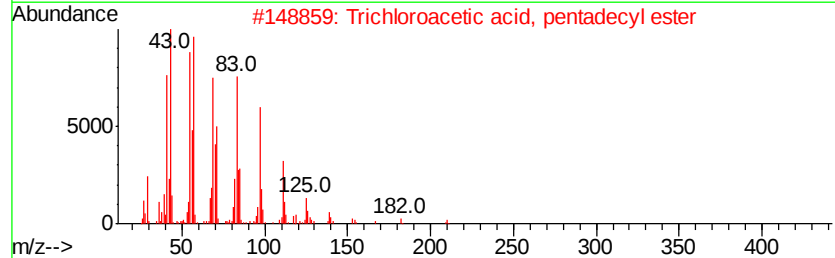
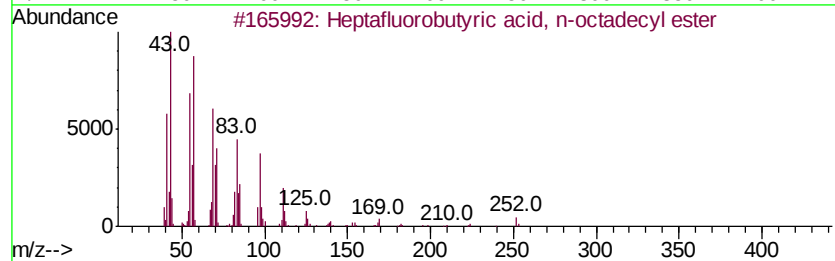
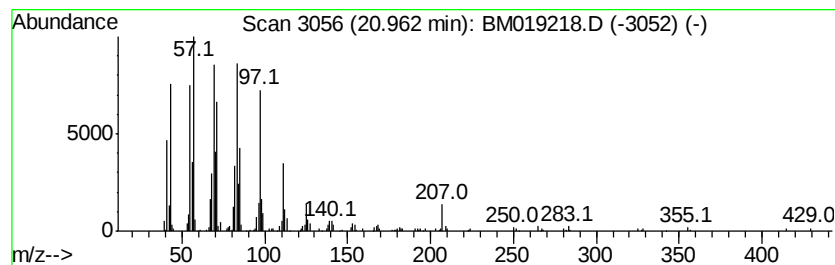
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.96	4.04 ng	535437	Chrysene-d12	21.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-octadecyl...	466	C22H37F7O2	000400-57-7	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4		1-Hexadecanol	242	C16H34O	036653-82-4	87
5		1-Heptadecanol	256	C17H36O	001454-85-9	87



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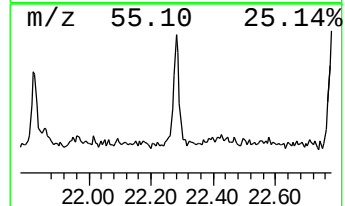
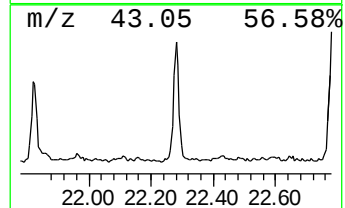
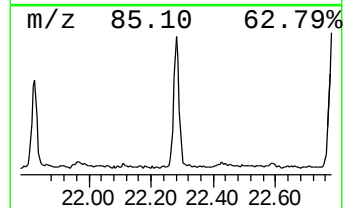
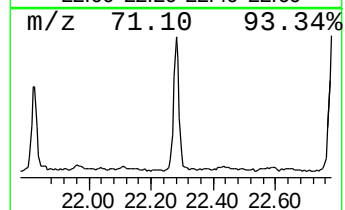
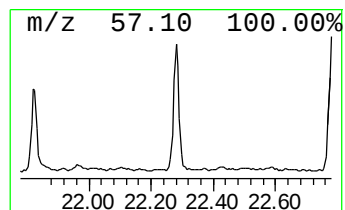
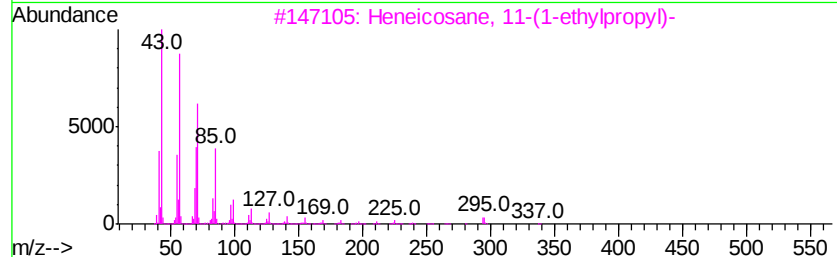
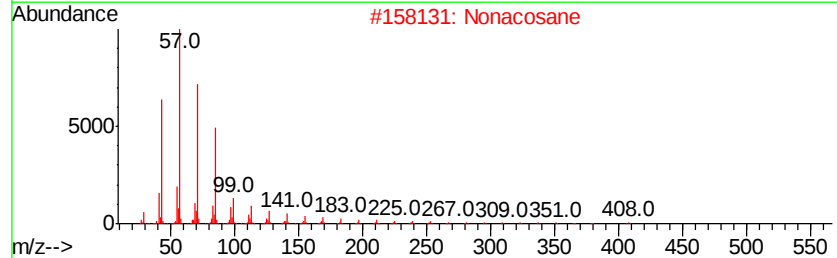
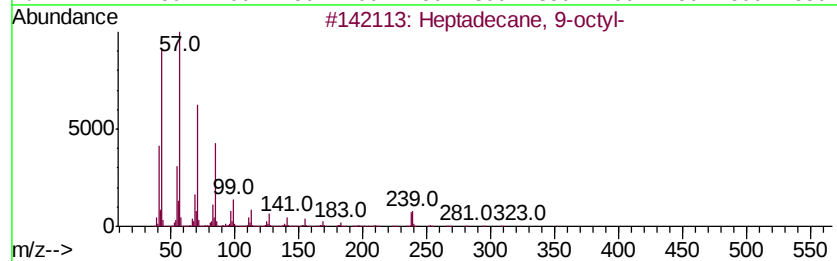
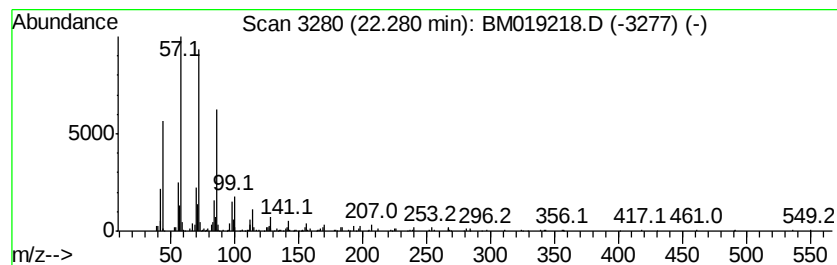
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	2.44 ng	323523	Chrysene-d12	21.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
2	Nonacosane	408 C29H60	000630-03-5	91
3	Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6	91
4	Heptacosane	380 C27H56	000593-49-7	91
5	Octadecane	254 C18H38	000593-45-3	83



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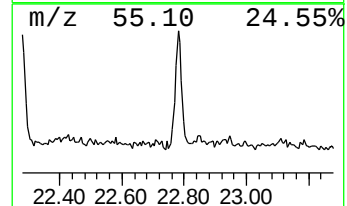
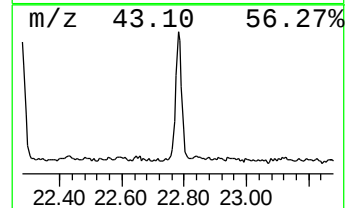
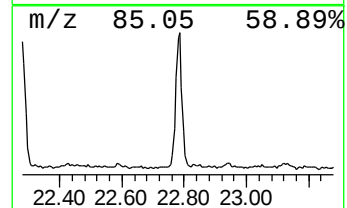
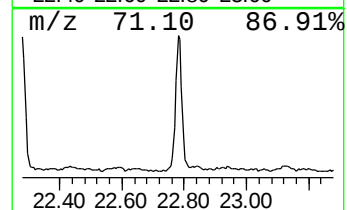
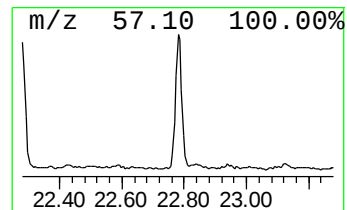
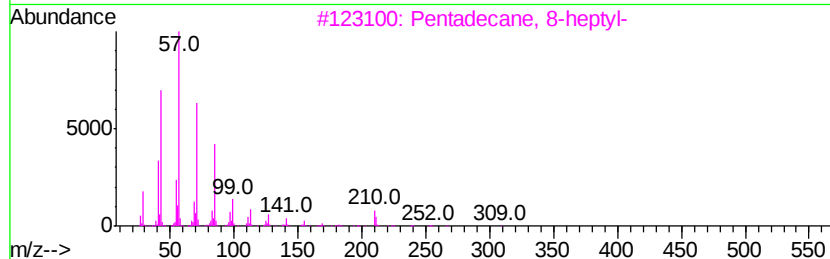
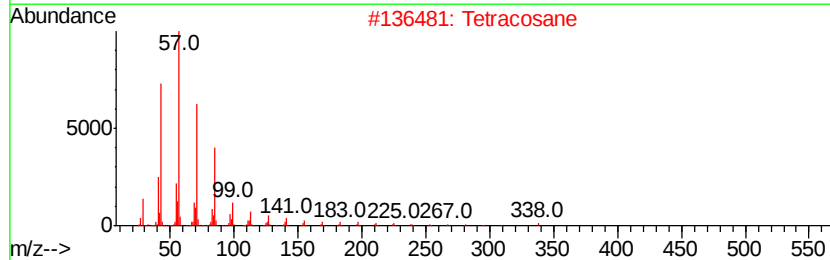
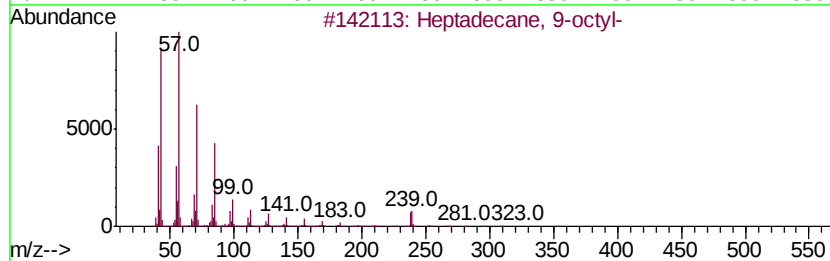
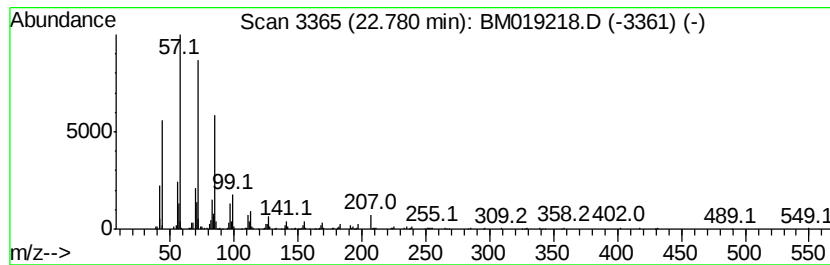
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.78	3.72 ng	415747	Perylene-d12	23.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5		Nonacosane	408	C29H60	000630-03-5	90



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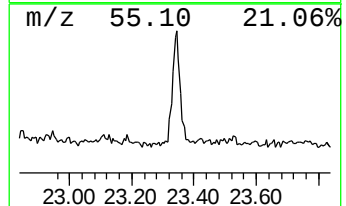
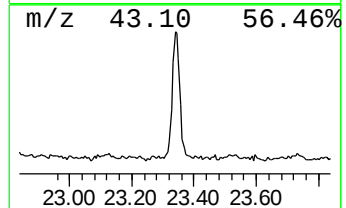
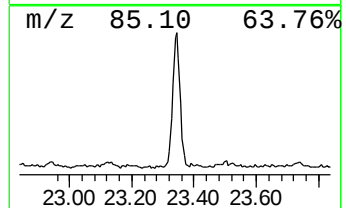
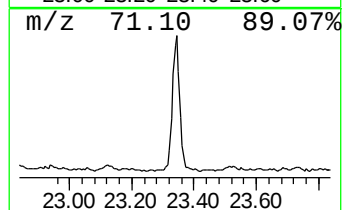
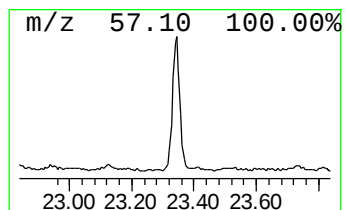
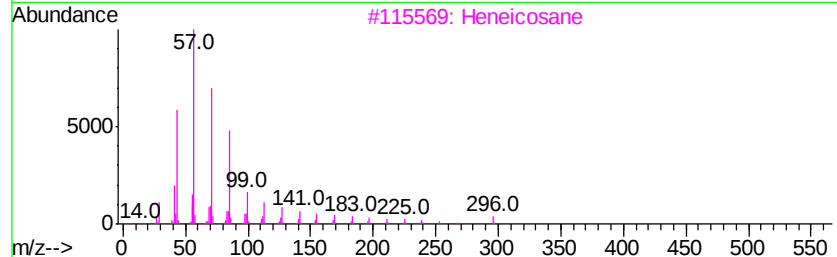
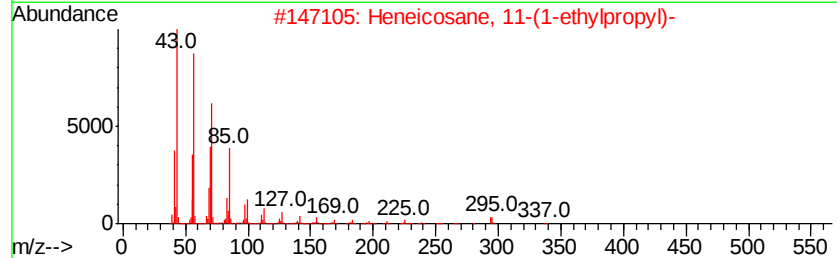
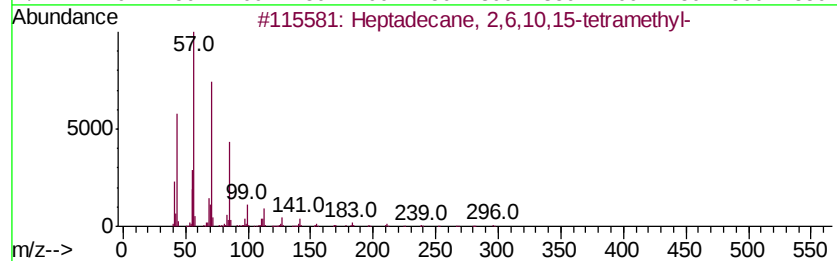
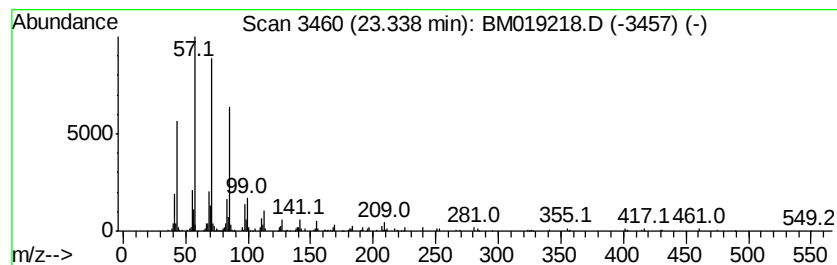
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	3.49 ng	390132	Perylene-d12	23.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
3		Heneicosane	296	C21H44	000629-94-7	86
4		10-Methylnonadecane	282	C20H42	056862-62-5	86
5		Octacosane	394	C28H58	000630-02-4	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM031819\
Data File : BM019218.D
Acq On : 18 Mar 2019 16:39
Operator : JU/SJ
Sample : K1935-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-17(0.5-1.5)

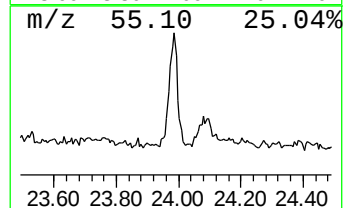
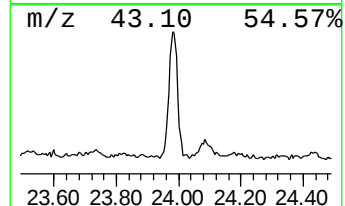
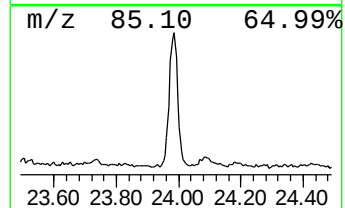
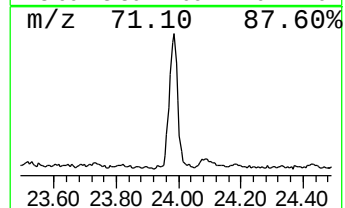
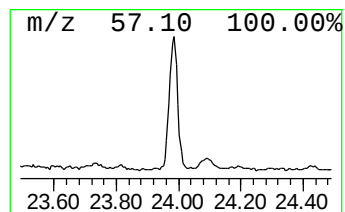
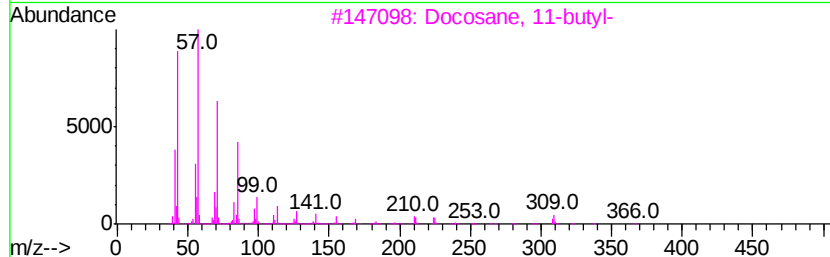
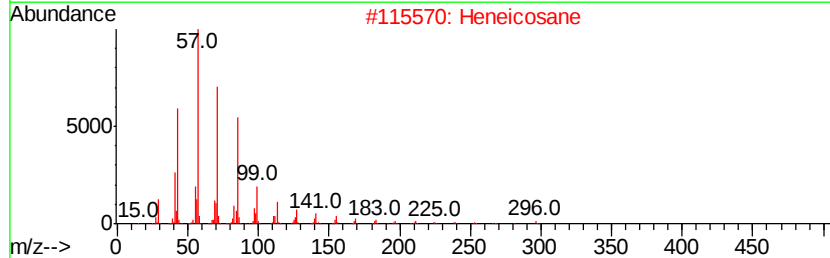
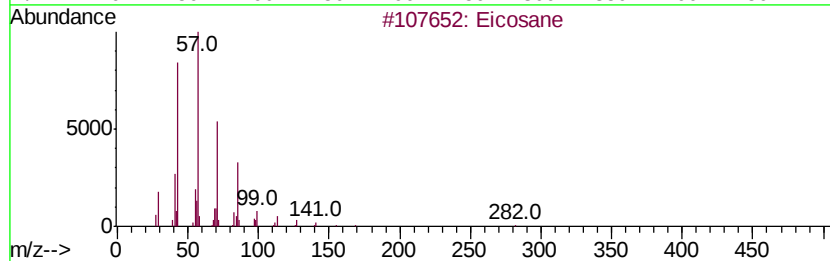
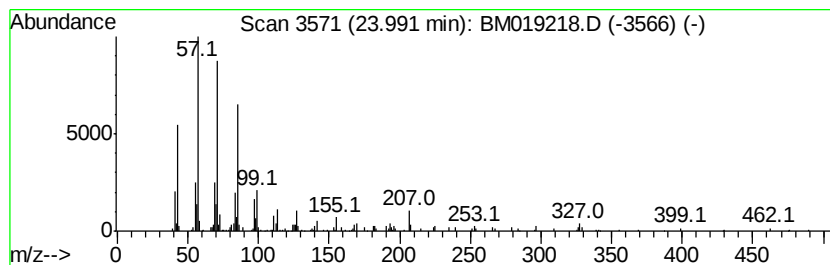
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	3.29 ng	367750	Perylene-d12	23.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Heneicosane		296	C21H44	000629-94-7	86
3	Docosane, 11-butyl-		366	C26H54	013475-76-8	86
4	Hexadecane		226	C16H34	000544-76-3	83
5	2-Thiopheneacetic acid, 4-tetrad...		338	C20H34O2S	1000280-67-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM031819\
Data File : BM019218.D
Acq On : 18 Mar 2019 16:39
Operator : JU/SJ
Sample : K1935-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-17(0.5-1.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.19	7.19	90.9	ng	5388870	1	7.65	1185560	20.0
n-Hexadecanoic acid	17.95	2.7	ng	396808	4	17.06	2914290	20.0
Heptafluorobutyri...	20.96	4.0	ng	535437	5	21.26	2651230	20.0
Heptadecane, 9-oc...	22.28	2.4	ng	323523	5	21.26	2651230	20.0
Tetracosane	22.78	3.7	ng	415747	6	23.49	2235310	20.0
Heptadecane, 2,6,...	23.34	3.5	ng	390132	6	23.49	2235310	20.0
Eicosane	23.99	3.3	ng	367750	6	23.49	2235310	20.0