

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030519\
 Data File : BM019059.D
 Acq On : 06 Mar 2019 06:05
 Operator : JU/SJ
 Sample : K1704-10
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PST-028-SW062-022719

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-BM021119.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	5.269	365	371	388	rBV	4480849	6457783	44.19%	7.332%
2	6.851	633	640	653	rBV	4402600	7141107	48.86%	8.108%
3	7.210	693	701	719	rBV	4565390	7334632	50.19%	8.327%
4	7.675	773	780	788	rBV	861371	1393286	9.53%	1.582%
5	7.986	826	833	845	rBV	3280600	5232281	35.80%	5.940%
6	8.839	970	978	1000	rBV	2416998	4225320	28.91%	4.797%
7	10.457	1246	1253	1267	rBV	1111677	1889530	12.93%	2.145%
8	12.939	1666	1675	1690	rBV	6687067	9647428	66.01%	10.953%
9	13.792	1813	1820	1831	rBV	281143	434945	2.98%	0.494%
10	14.327	1904	1911	1926	rVB2	1538219	2450913	16.77%	2.783%
11	15.827	2159	2166	2183	rBV	5584188	7969531	54.53%	9.048%
12	17.080	2373	2379	2384	rBV	2100266	2987895	20.44%	3.392%
13	17.968	2524	2530	2541	rBV	873372	1387267	9.49%	1.575%
14	19.145	2725	2730	2736	rVB	171973	253492	1.73%	0.288%
15	19.256	2744	2749	2762	rBV	277309	484728	3.32%	0.550%
16	19.509	2788	2792	2800	rVB	140194	215838	1.48%	0.245%
17	19.715	2821	2827	2840	rBV	11743753	14614629	100.00%	16.593%
18	20.974	3037	3041	3052	rBV	1723899	2159549	14.78%	2.452%
19	21.274	3087	3092	3097	rBV	2845836	3865804	26.45%	4.389%
20	21.421	3113	3117	3122	rBV4	119158	216311	1.48%	0.246%
21	21.868	3187	3193	3204	rBV	928014	1501922	10.28%	1.705%
22	22.433	3285	3289	3295	rVB	835279	1060816	7.26%	1.204%
23	22.809	3350	3353	3356	rBV	196875	236528	1.62%	0.269%
24	22.862	3358	3362	3373	rVB2	427666	780927	5.34%	0.887%
25	23.521	3468	3474	3486	rVB	1824481	3448729	23.60%	3.915%
26	24.115	3571	3575	3586	rVB2	332306	687802	4.71%	0.781%

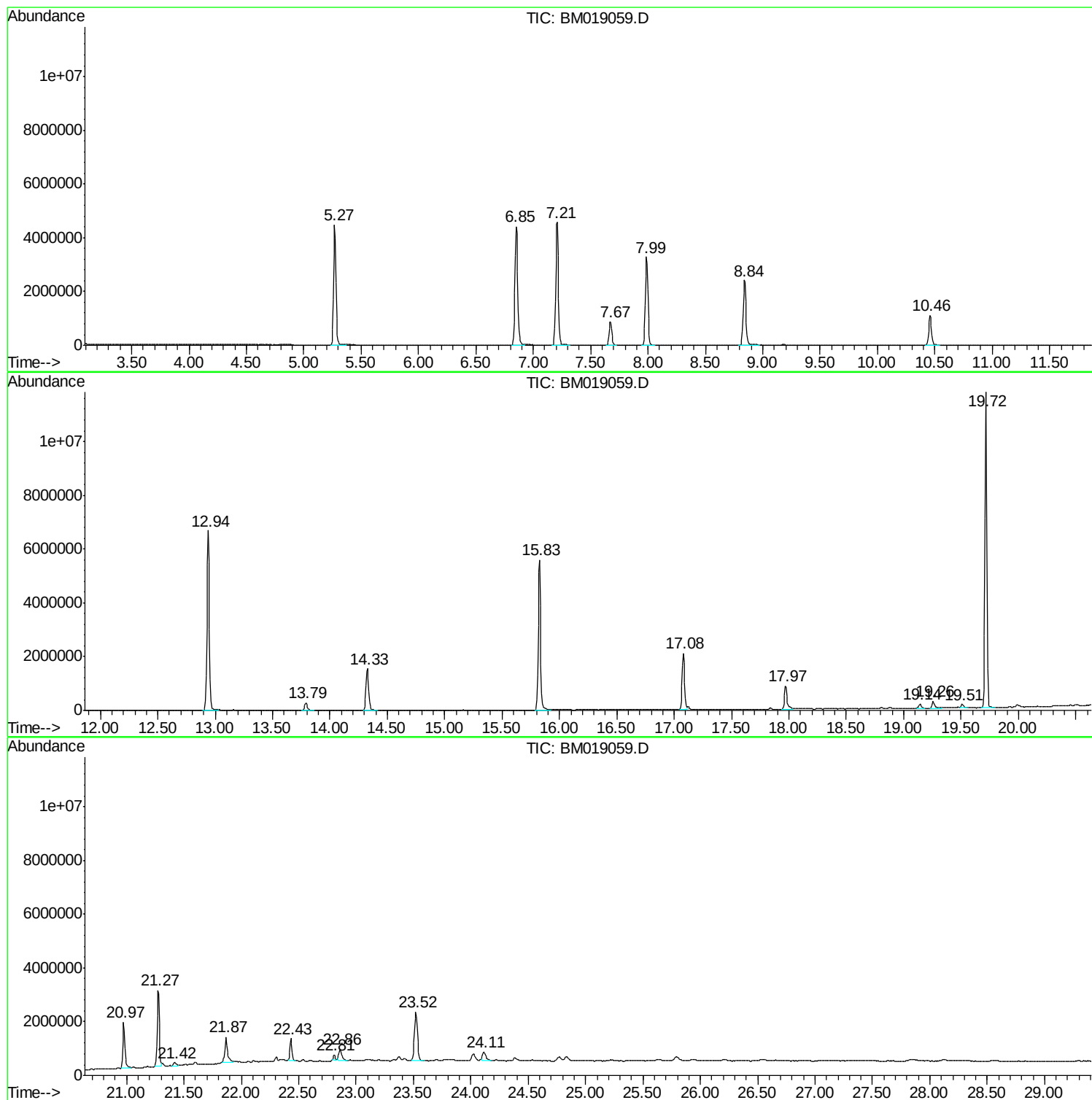
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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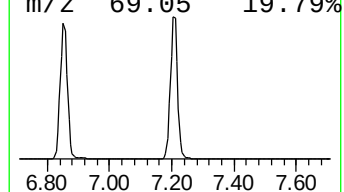
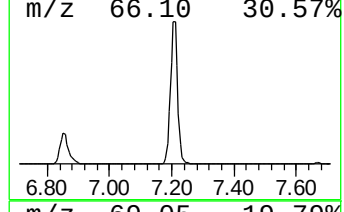
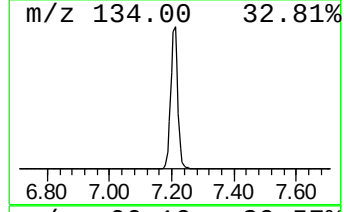
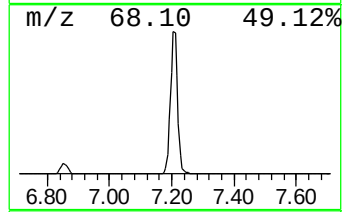
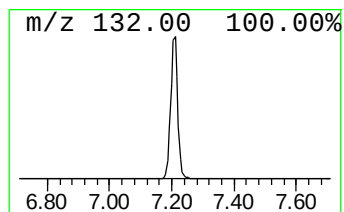
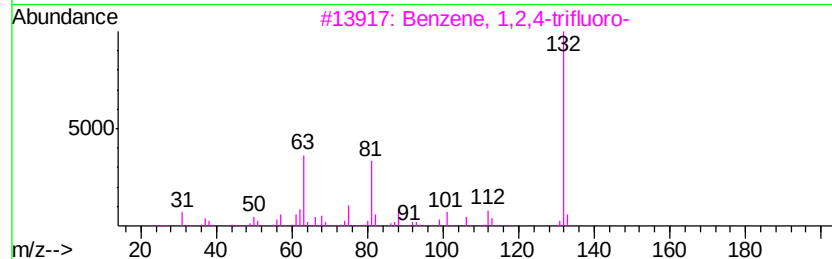
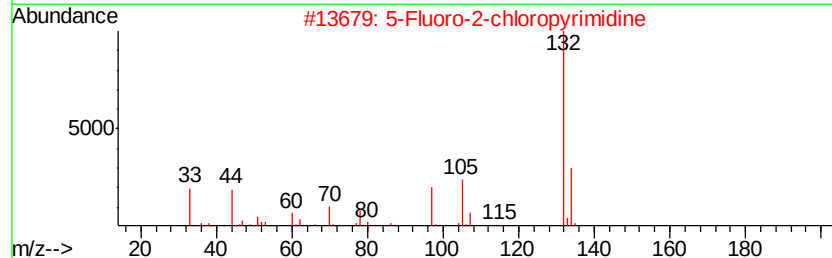
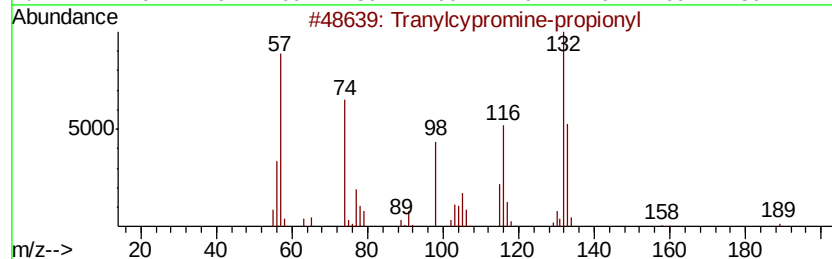
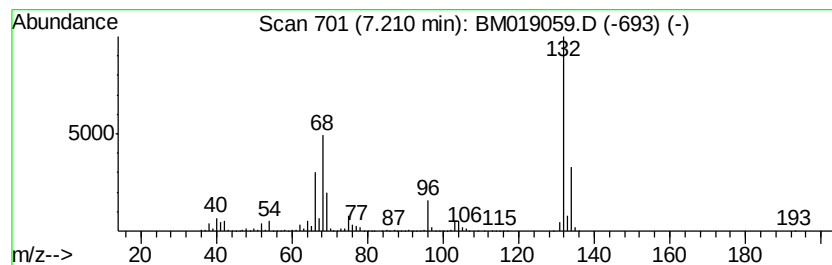
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	105.29 ng	7334630	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcyppromine-propionyl	189	C12H15NO	1000123-86-3	12
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
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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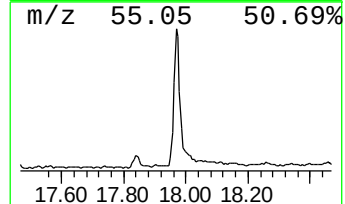
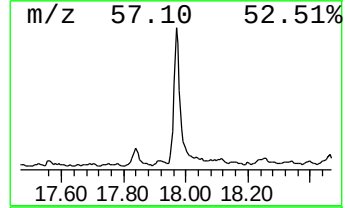
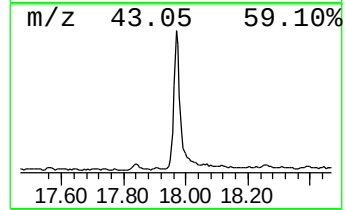
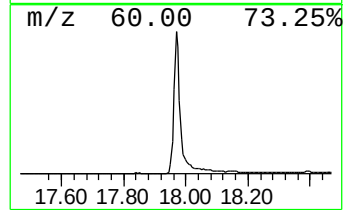
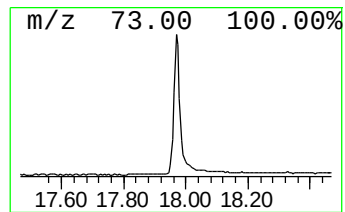
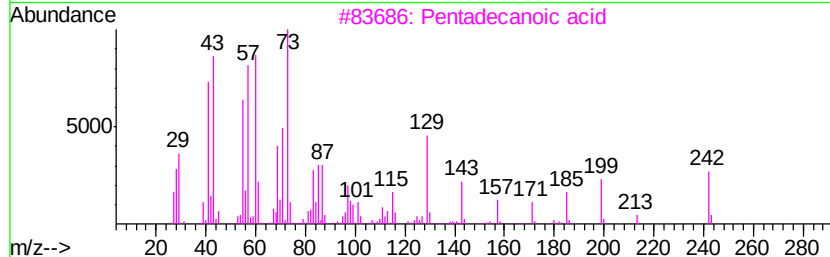
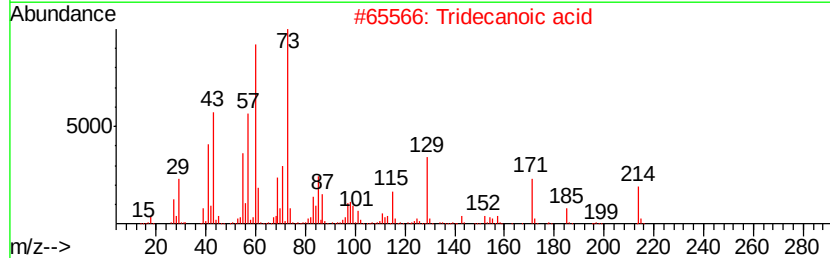
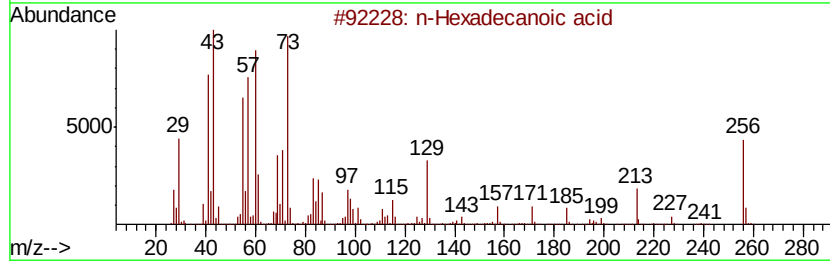
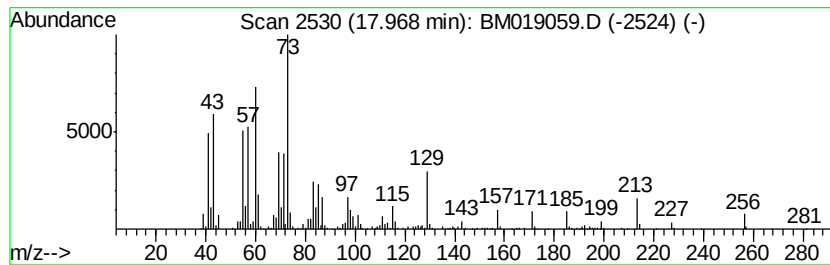
Instrument :
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.97	9.29 ng	1387270	Phenanthrene-d10	17.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Sedoheptulosan	192	C7H12O6	000469-90-9	35
5	Tridecane, 4-methyl-	198	C14H30	026730-12-1	15



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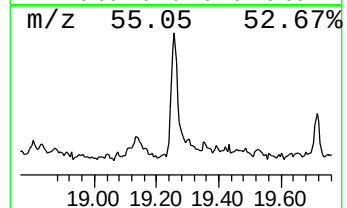
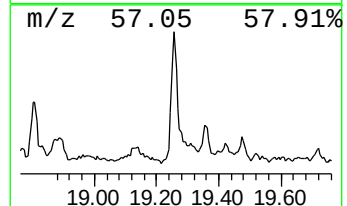
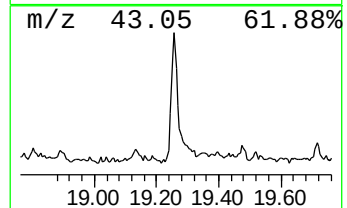
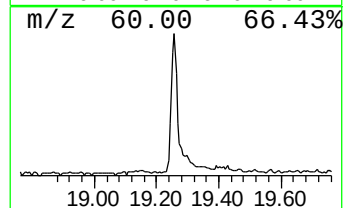
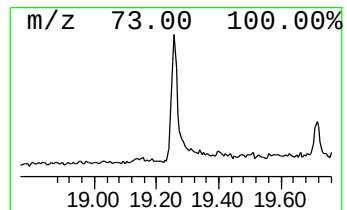
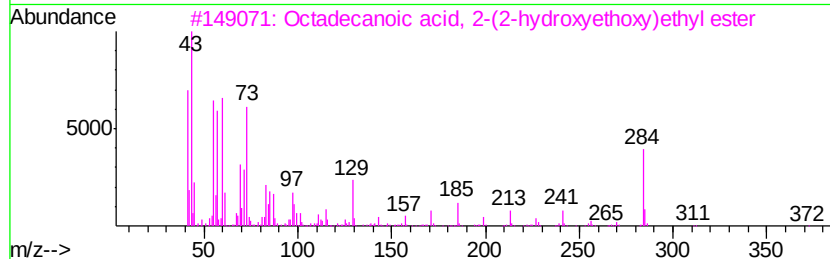
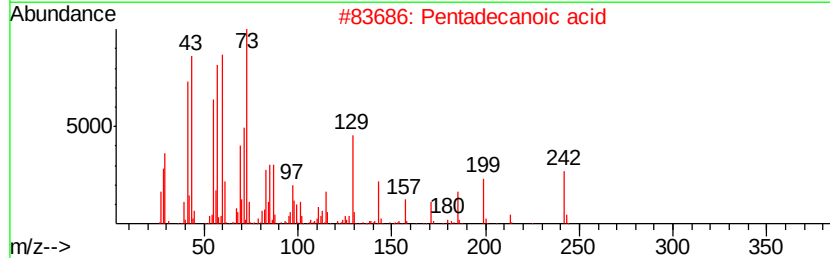
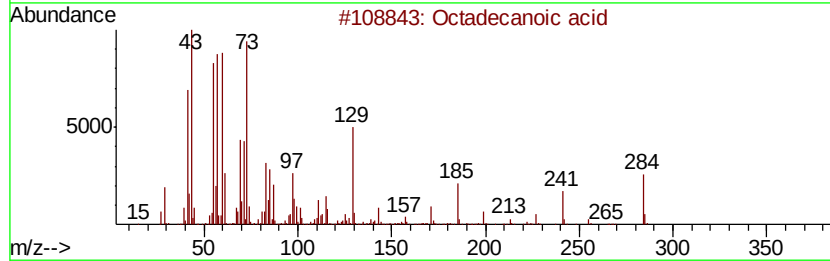
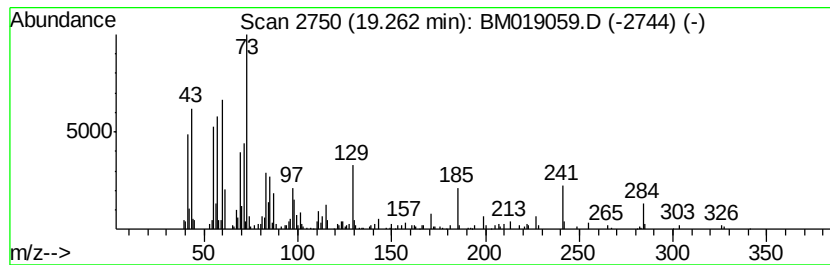
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Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	2.51 ng	484728	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	86
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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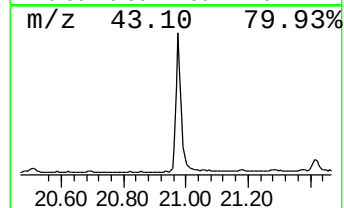
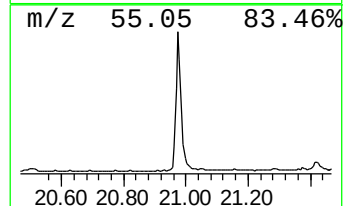
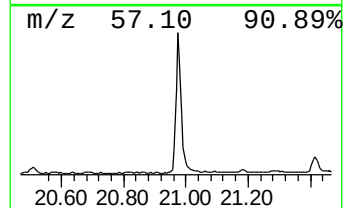
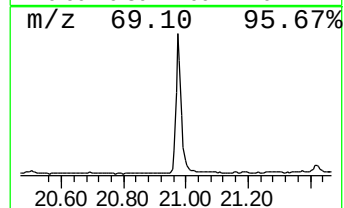
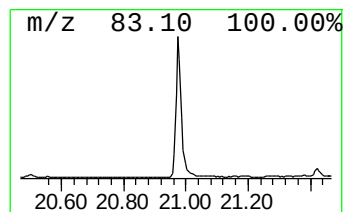
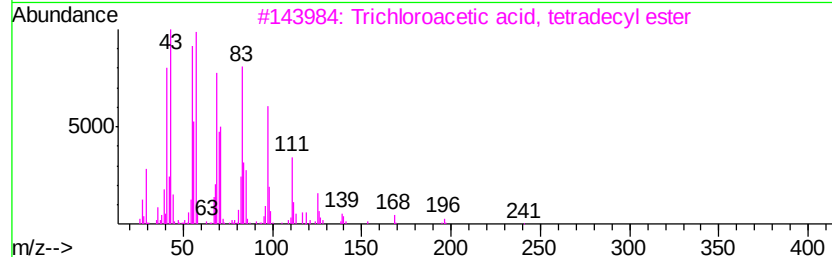
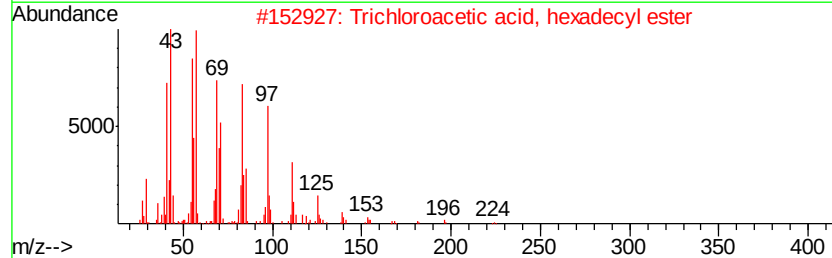
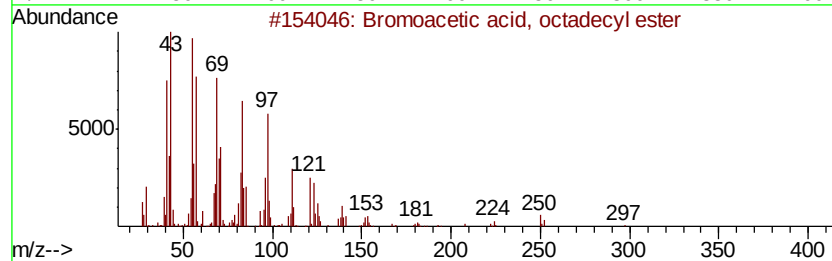
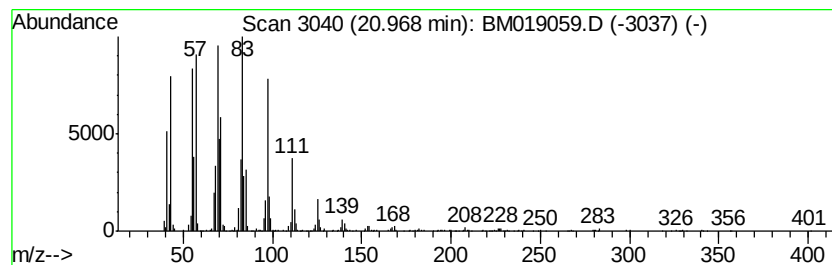
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Peak Number 5 Bromoacetic acid, octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	11.17 ng	2159550	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91



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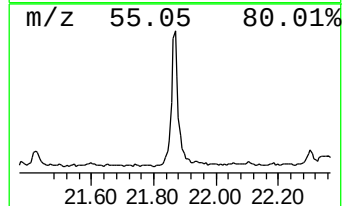
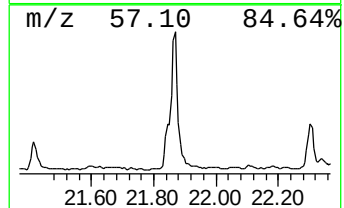
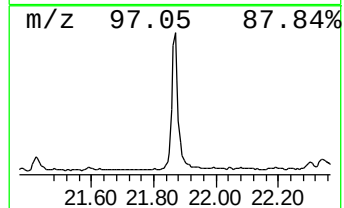
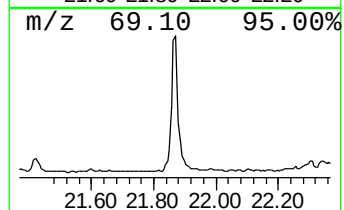
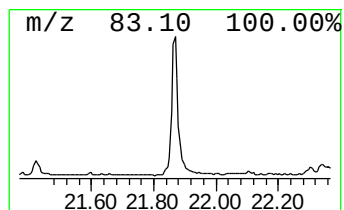
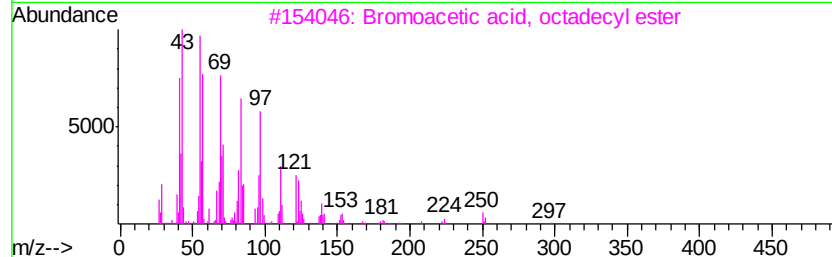
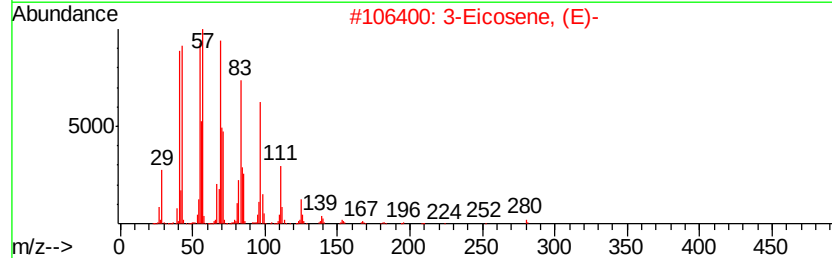
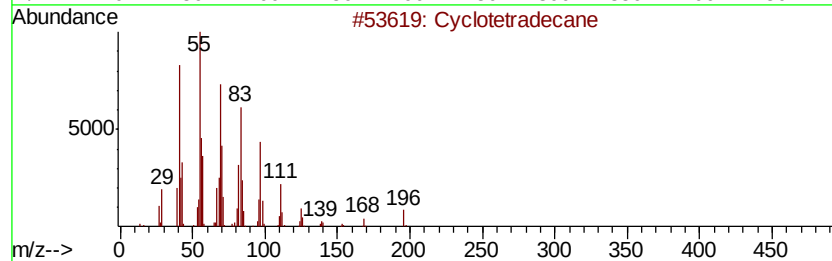
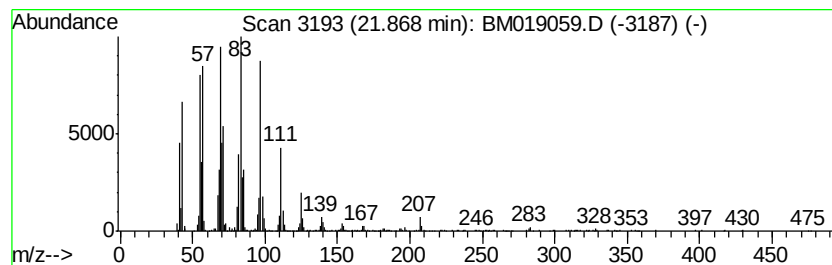
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.87	7.77 ng	1501920	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetradecane	196	C14H28	000295-17-0	93
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4		Cyclotetracosane	336	C24H48	000297-03-0	91
5		1-Heptadecanol	256	C17H36O	001454-85-9	90



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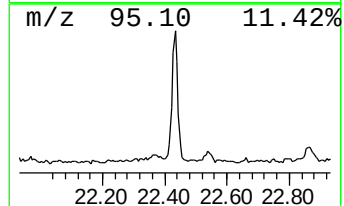
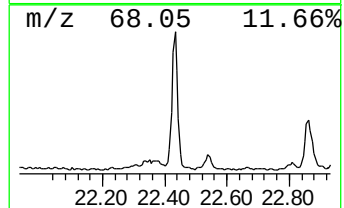
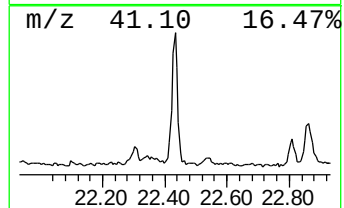
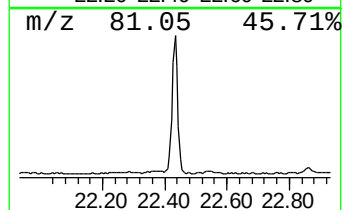
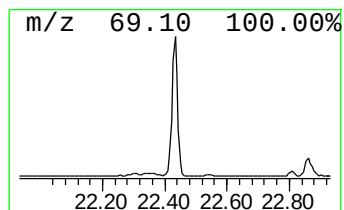
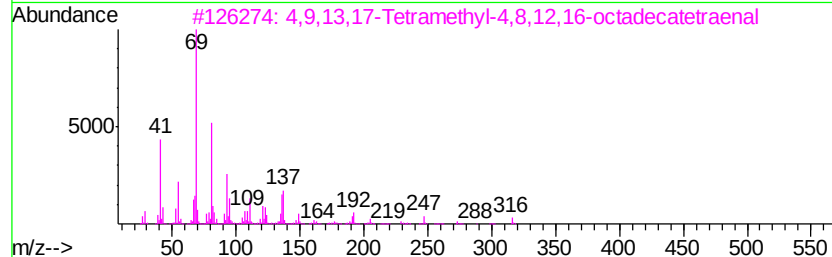
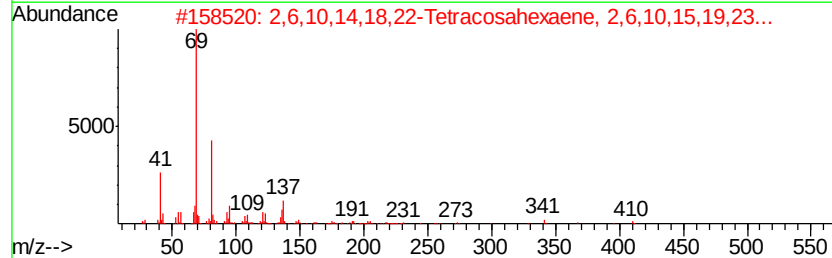
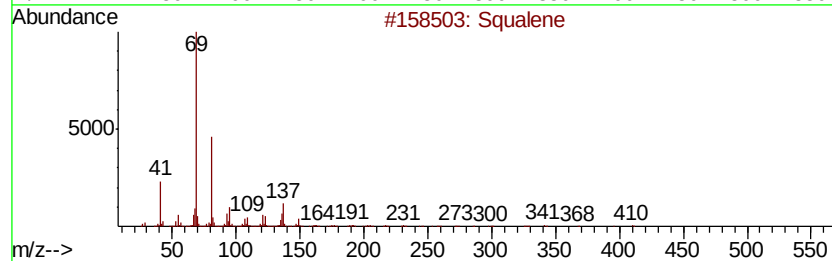
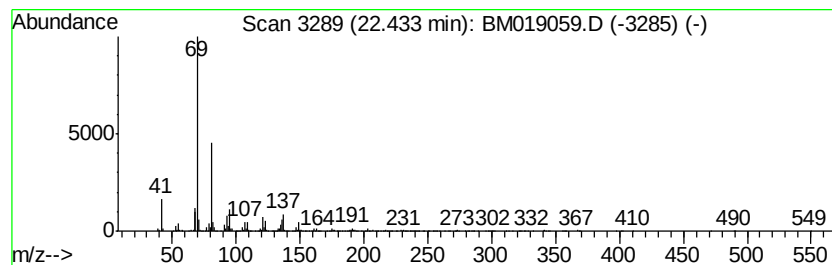
Instrument :
BNA_M
ClientSampleId :
PST-028-SW062-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.43	6.15 ng	1060820	Perylene-d12	23.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	91
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H360	056882-09-8	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H240	125529-10-4	72
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203 C12H17N3	003974-79-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030519\
Data File : BM019059.D
Acq On : 06 Mar 2019 06:05
Operator : JU/SJ
Sample : K1704-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

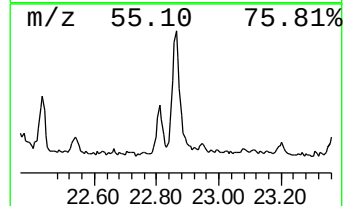
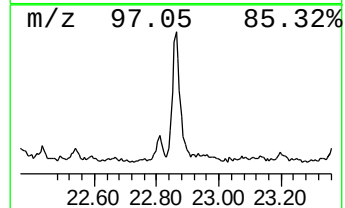
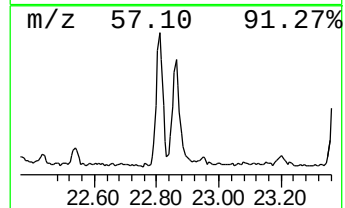
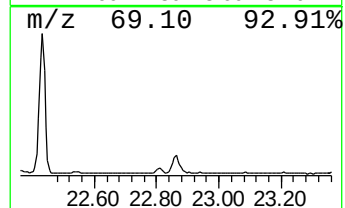
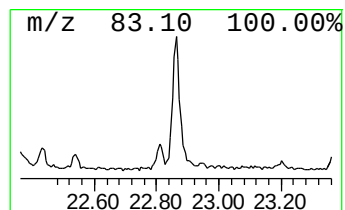
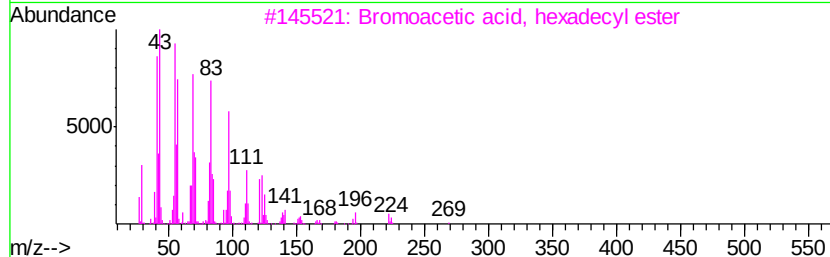
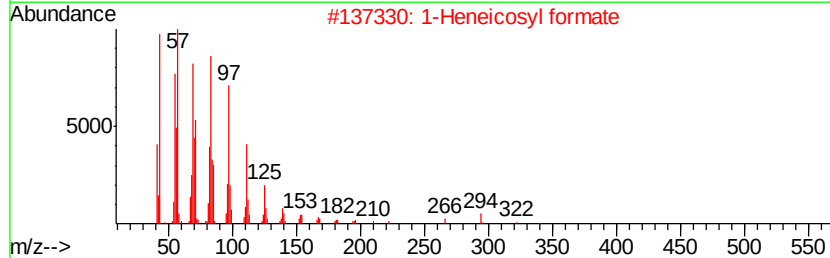
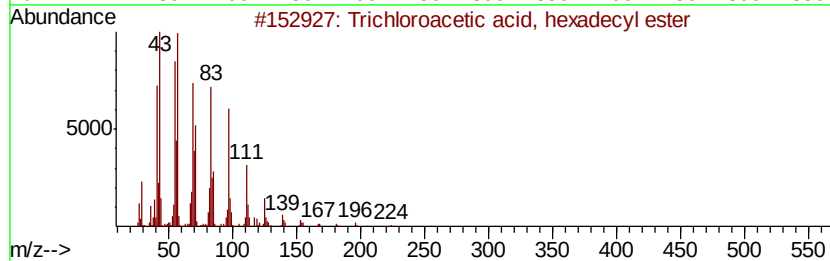
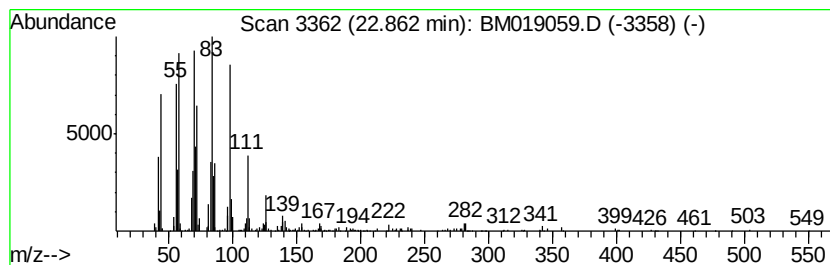
Instrument :
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ClientSampleId :
PST-028-SW062-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.86	4.53 ng	780927	Perylene-d12	23.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
4	Cyclotetradecane	196	C14H28	000295-17-0	74
5	1-Pentadecene	210	C15H30	013360-61-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030519\
Data File : BM019059.D
Acq On : 06 Mar 2019 06:05
Operator : JU/SJ
Sample : K1704-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

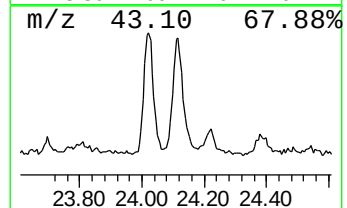
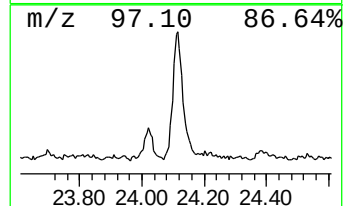
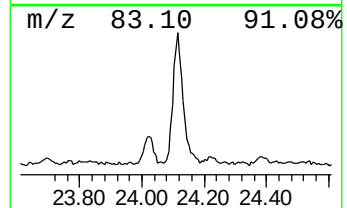
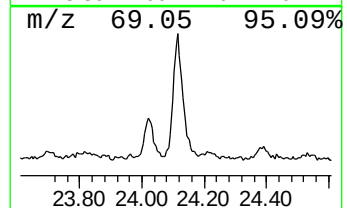
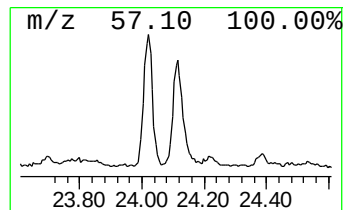
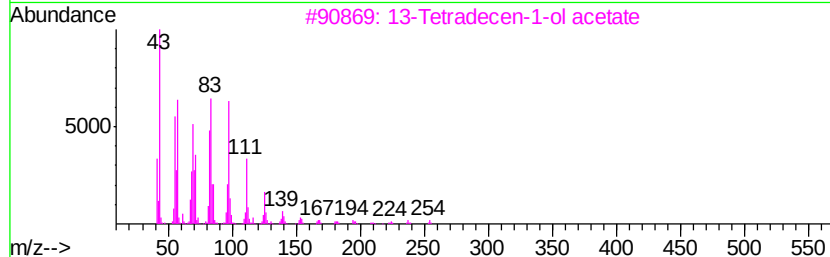
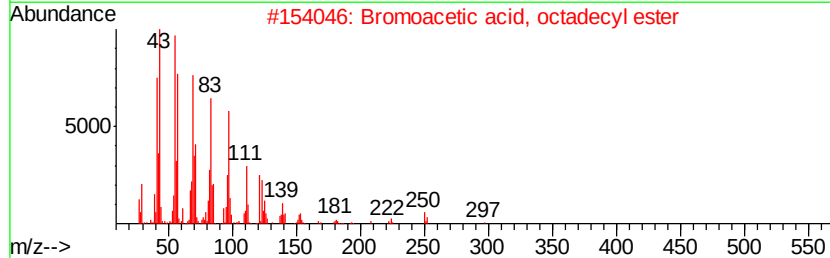
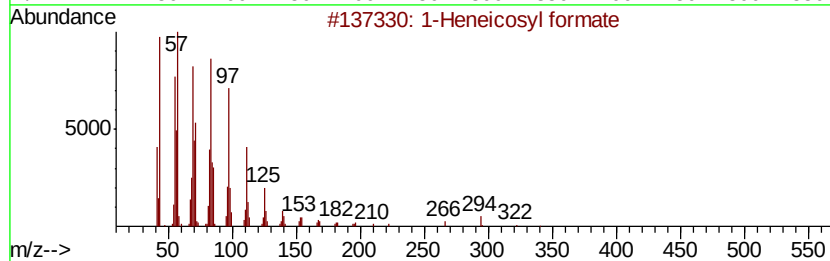
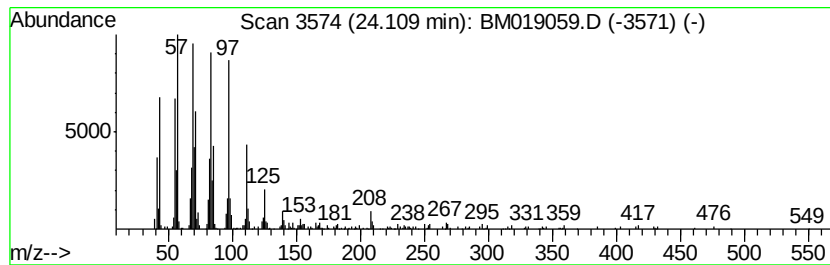
Instrument :
BNA_M
ClientSampleId :
PST-028-SW062-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosyl formate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.11	3.99 ng	687802	Perylene-d12	23.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosyl formate	340 C22H44O2	077899-03-7	89
2	Bromoacetic acid, octadecyl ester	390 C20H39BrO2	018992-03-5	87
3	13-Tetradecen-1-ol acetate	254 C16H30O2	056221-91-1	68
4	1-Triacontanol	438 C30H62O	000593-50-0	64
5	1-Eicosanol	298 C20H42O	000629-96-9	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030519\
Data File : BM019059.D
Acq On : 06 Mar 2019 06:05
Operator : JU/SJ
Sample : K1704-10
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PST-028-SW062-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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
unknown7.21	7.21	105.3	ng	7334630	1	7.67	1393290	20.0
n-Hexadecanoic acid	17.97	9.3	ng	1387270	4	17.08	2987900	20.0
Octadecanoic acid	19.26	2.5	ng	484728	5	21.27	3865800	20.0
Bromoacetic acid,...	20.97	11.2	ng	2159550	5	21.27	3865800	20.0
Cyclotetradecane	21.87	7.8	ng	1501920	5	21.27	3865800	20.0
Squalene	22.43	6.2	ng	1060820	6	23.52	3448730	20.0
Trichloroacetic a...	22.86	4.5	ng	780927	6	23.52	3448730	20.0
1-Heneicosyl formate	24.11	4.0	ng	687802	6	23.52	3448730	20.0