

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
 Data File : BG043492.D
 Acq On : 4 Nov 2019 22:19
 Operator : JU
 Sample : K5676-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SU-02-110119

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_G\METHODS\8270-BG102119.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	3.173	9	14	25	rVB	82988	131355	6.04%	0.869%
2	5.112	338	344	355	rBV2	78826	126170	5.80%	0.835%
3	5.594	419	426	443	rBV	370761	659139	30.30%	4.361%
4	7.192	689	698	722	rBV	385372	792620	36.44%	5.244%
5	7.551	752	759	769	rBV	420288	756330	34.77%	5.004%
6	8.009	828	837	847	rBV	122630	219812	10.11%	1.454%
7	8.332	883	892	902	rBV	311399	573367	26.36%	3.794%
8	9.172	1028	1035	1051	rBV	200144	435644	20.03%	2.882%
9	10.817	1304	1315	1326	rBV	139628	293314	13.48%	1.941%
10	13.262	1724	1731	1743	rBV	673714	1151218	52.92%	7.617%
11	14.090	1866	1872	1887	rBV2	67776	132938	6.11%	0.880%
12	14.636	1957	1965	1977	rBV	283475	489413	22.50%	3.238%
13	16.129	2211	2219	2240	rBV	692170	1191383	54.77%	7.883%
14	17.386	2426	2433	2448	rBV	374178	658460	30.27%	4.357%
15	17.504	2448	2453	2459	rVB7	13167	23106	1.06%	0.153%
16	18.044	2539	2545	2555	rBV	290258	379057	17.43%	2.508%
17	18.273	2579	2584	2594	rBV3	61110	119029	5.47%	0.788%
18	19.184	2733	2739	2741	rBV	744194	969556	44.57%	6.415%
19	19.213	2741	2744	2757	rVV2	1275526	1644441	75.60%	10.880%
20	19.343	2760	2766	2770	rBV2	127010	156073	7.18%	1.033%
21	19.437	2778	2782	2789	rBV2	29192	48239	2.22%	0.319%
22	19.801	2840	2844	2852	rVB	27971	52807	2.43%	0.349%
23	19.995	2871	2877	2891	rBV	1598584	2175199	100.00%	14.392%
24	20.436	2948	2952	2955	rBV6	26932	38843	1.79%	0.257%
25	21.293	3094	3098	3106	rBV4	89750	163915	7.54%	1.085%
26	21.652	3153	3159	3169	rBV	449137	797008	36.64%	5.273%
27	24.854	3695	3704	3715	rVB2	331484	935606	43.01%	6.190%

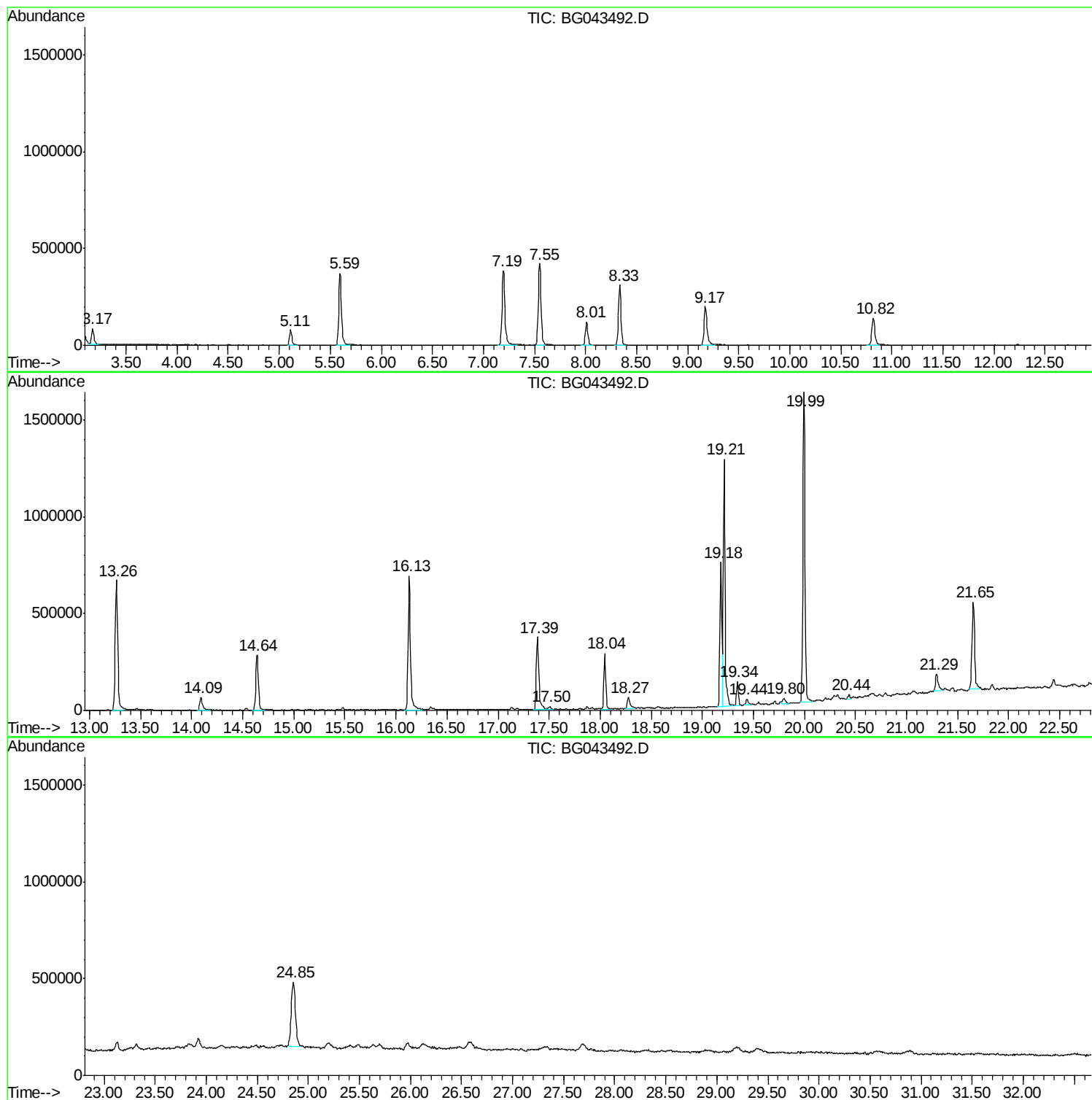
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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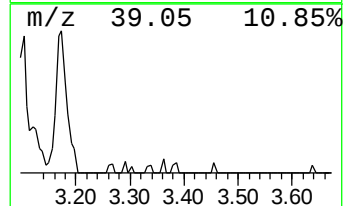
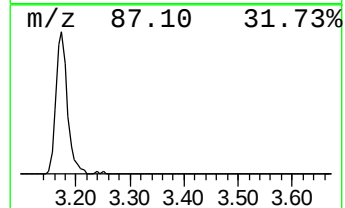
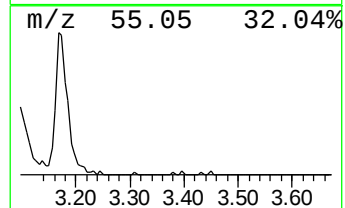
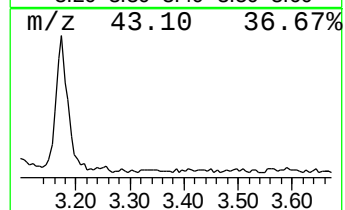
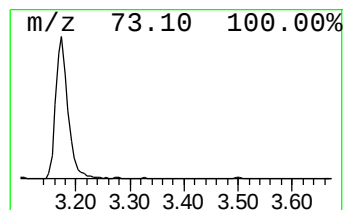
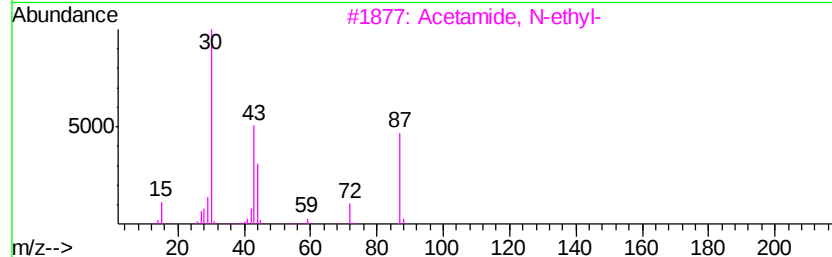
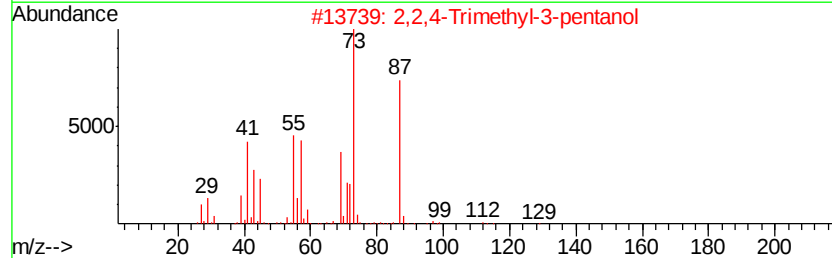
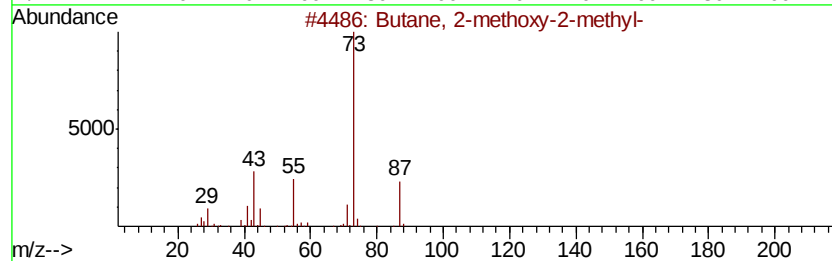
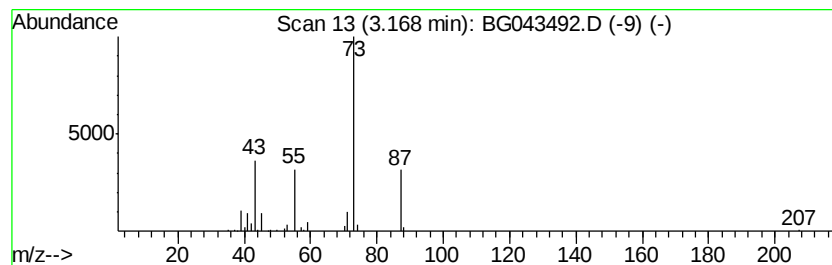
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	11.95 ng	131355	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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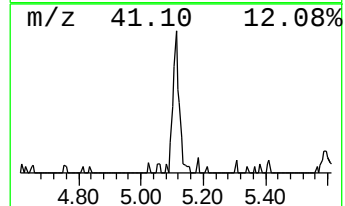
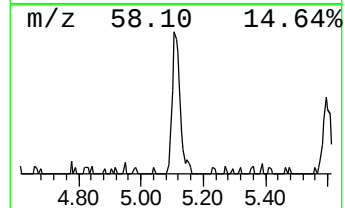
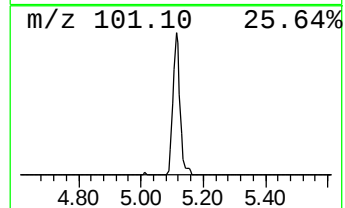
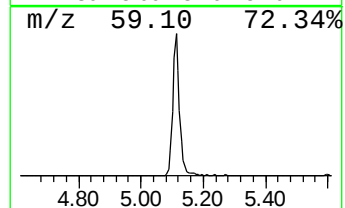
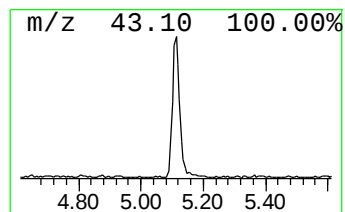
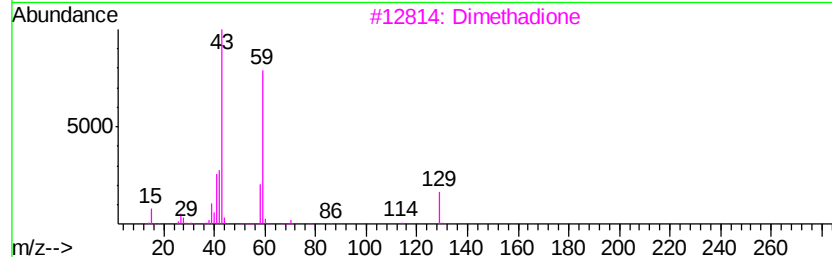
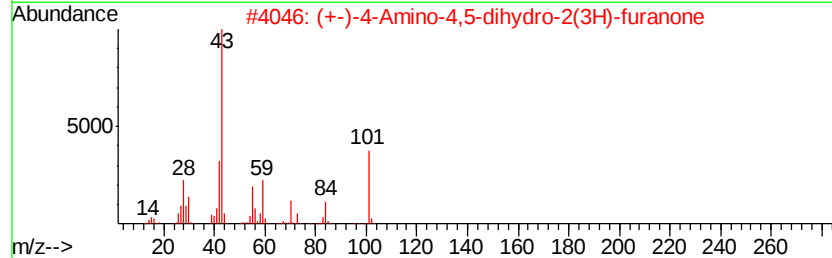
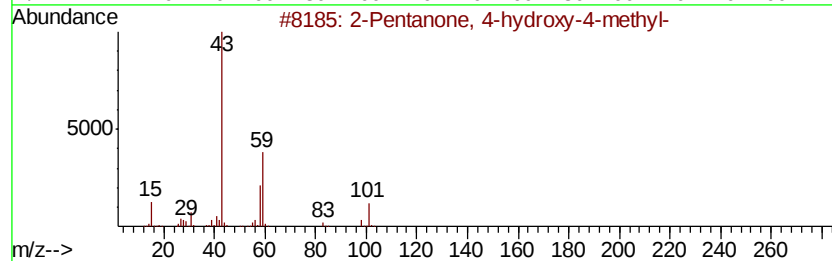
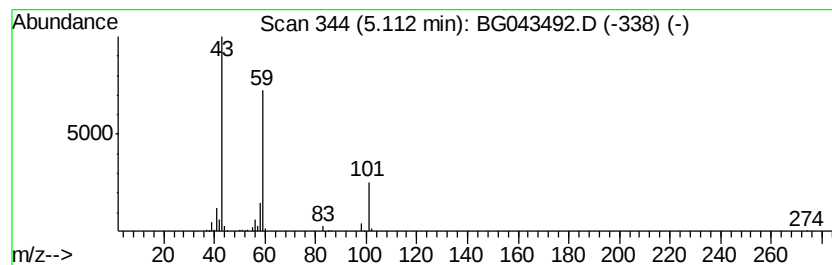
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	11.48 ng	126170	1,4-Dichlorobenzene-d4	8.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	64
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2		016504-58-8	43
3	Dimethadione	129	C5H7NO3		000695-53-4	33
4	Succinic acid, heptyl 2-methoxye...	274	C14H26O5		1000325-80-7	33
5	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	25



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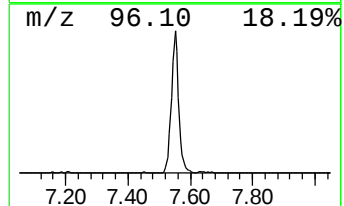
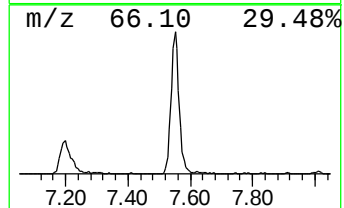
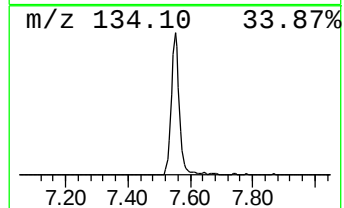
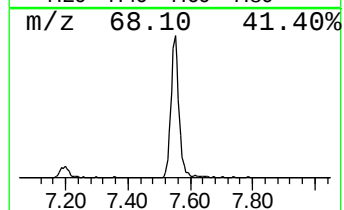
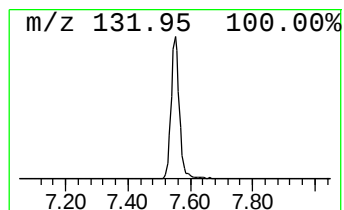
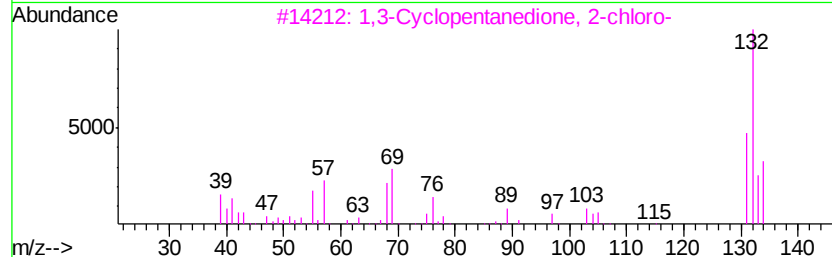
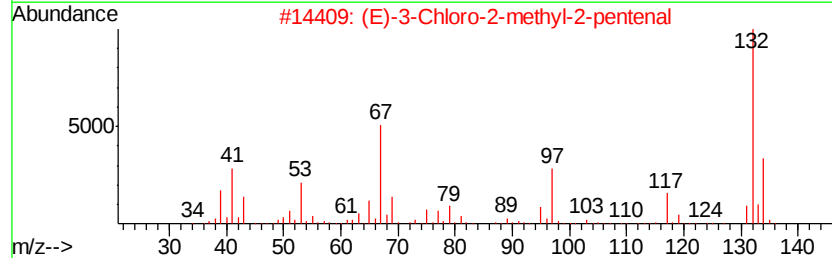
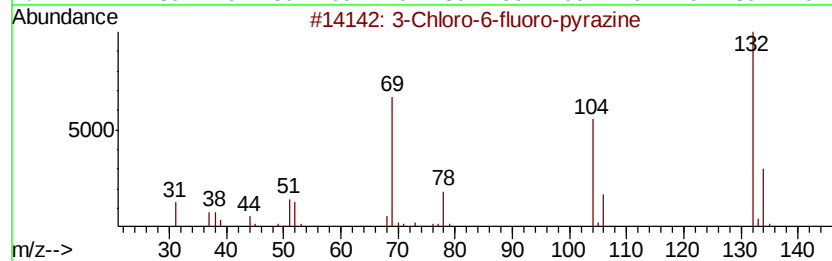
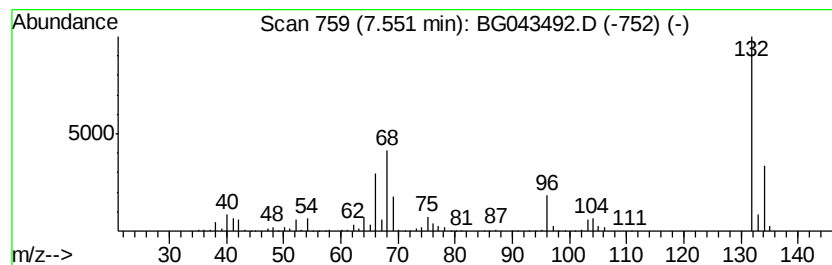
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Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	68.82 ng	756330	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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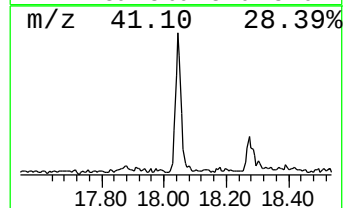
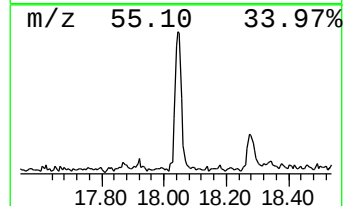
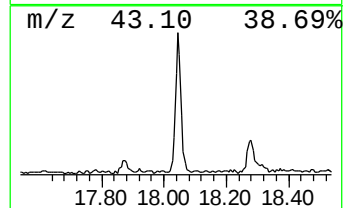
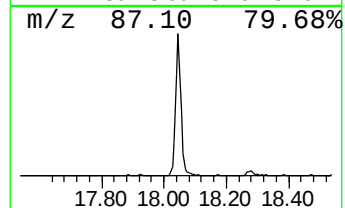
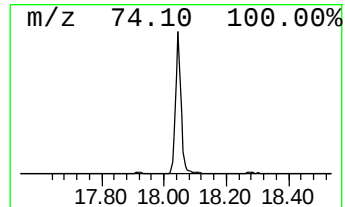
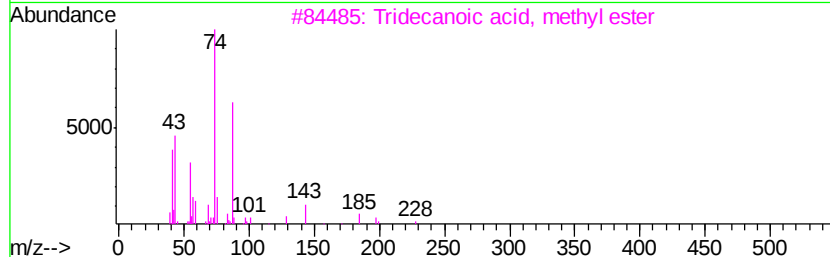
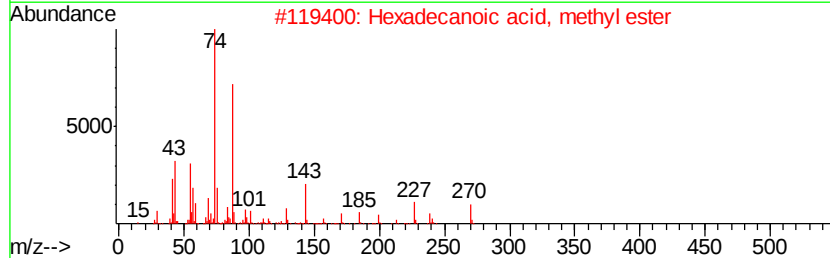
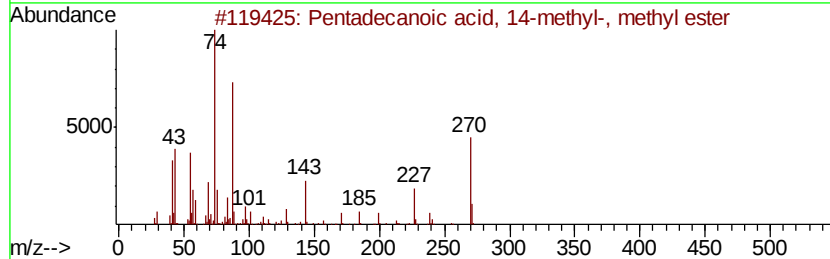
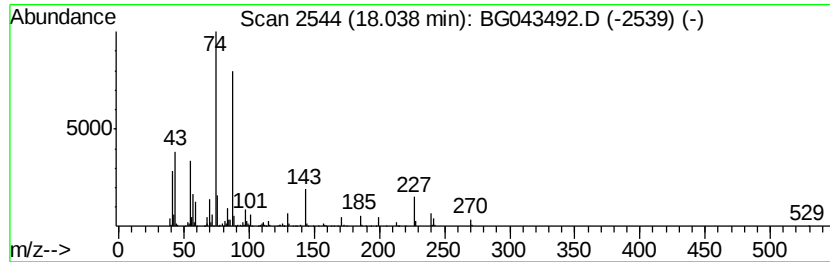
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Peak Number 5 Pentadecanoic acid, 14-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	11.51 ng	379057	Phenanthrene-d10	17.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
2		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
3		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4		Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	91
5		Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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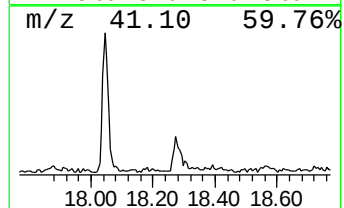
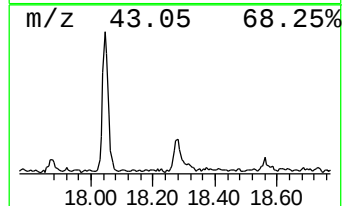
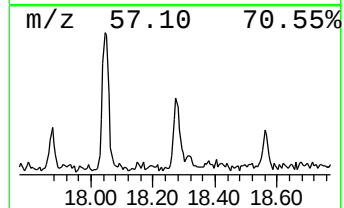
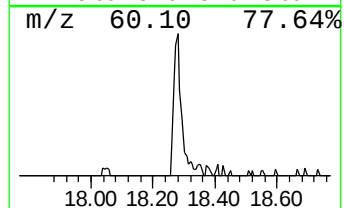
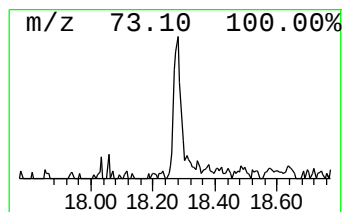
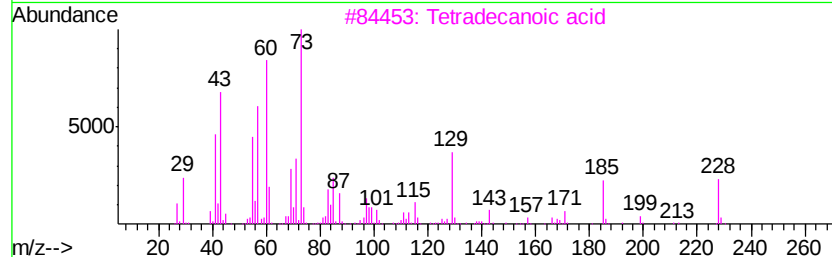
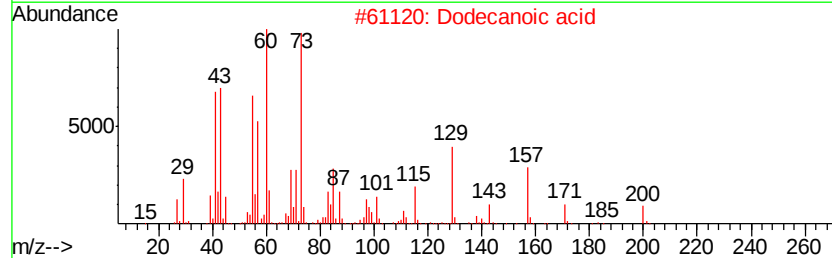
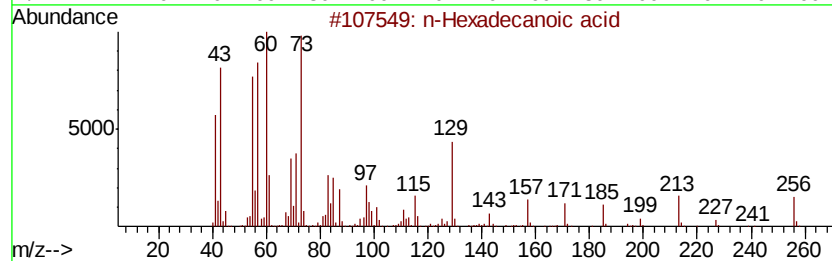
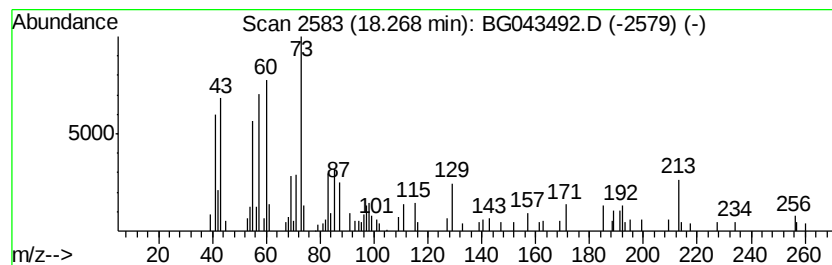
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.27	3.62 ng	119029	Phenanthrene-d10	17.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50



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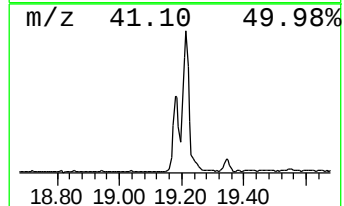
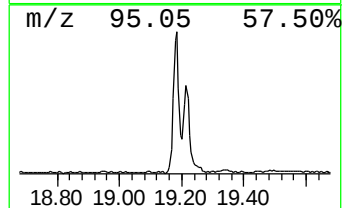
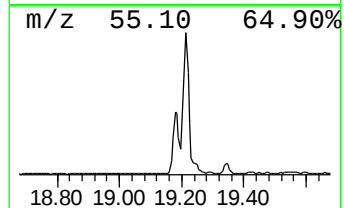
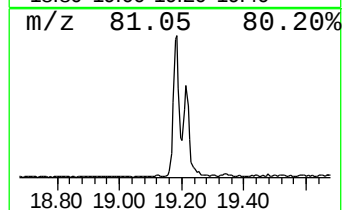
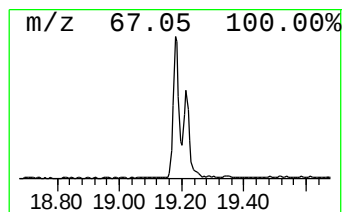
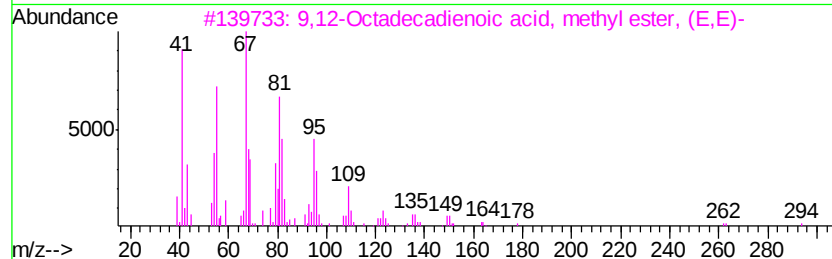
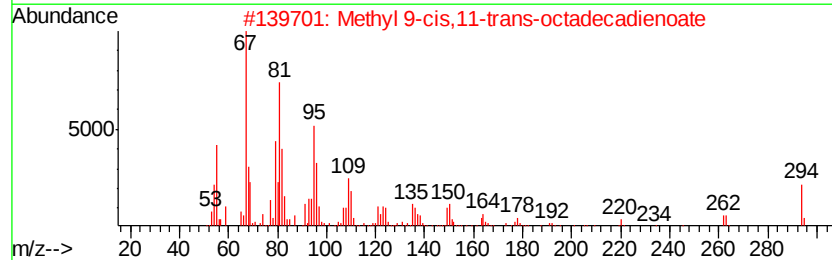
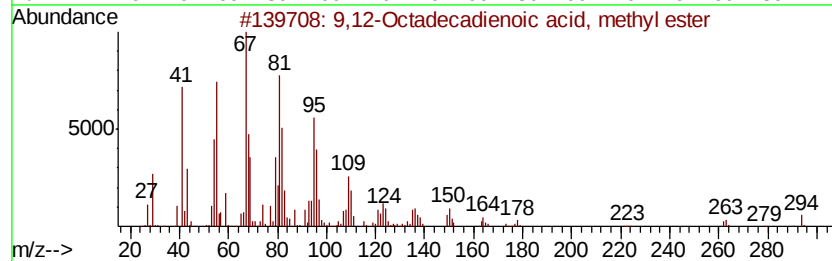
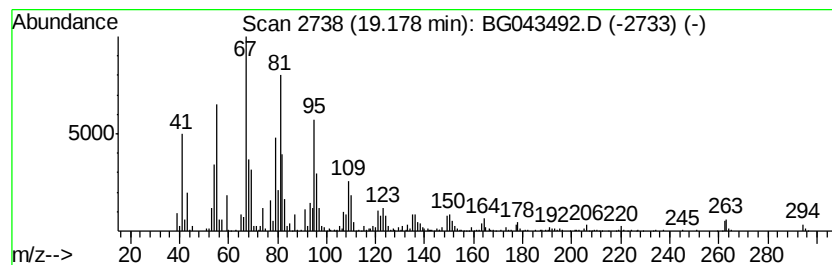
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BNA_G
ClientSampleId :
SU-02-110119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.18	29.45 ng	969556	Phenanthrene-d10	17.39		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99	
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99	
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99	
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99	
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99	



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
Data File : BG043492.D
Acq On : 4 Nov 2019 22:19
Operator : JU
Sample : K5676-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-02-110119

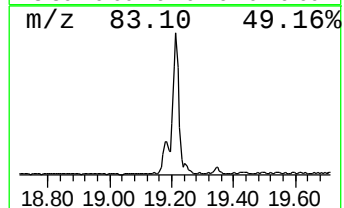
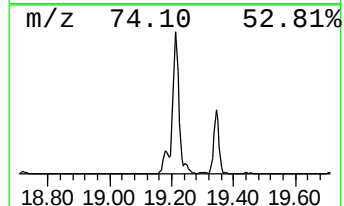
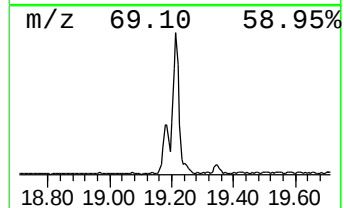
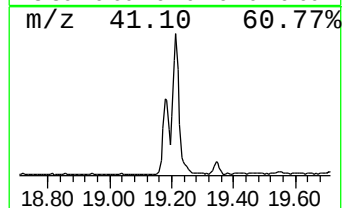
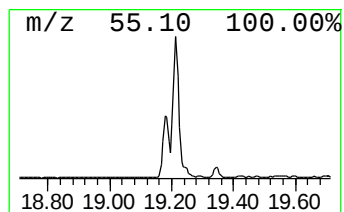
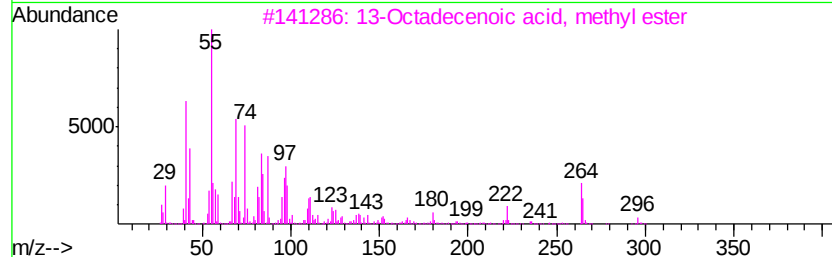
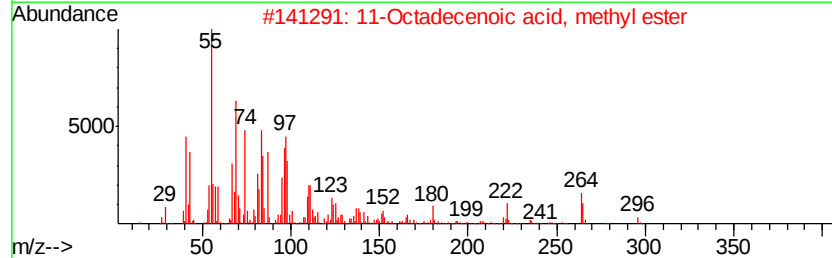
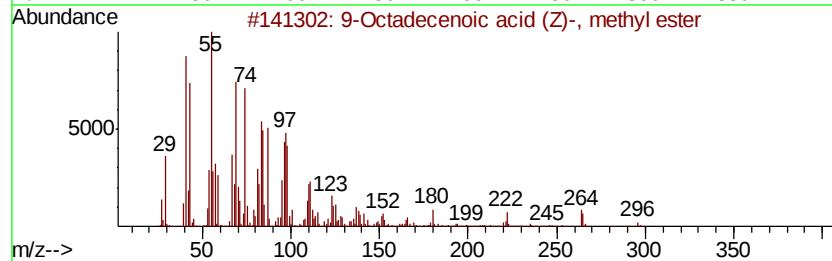
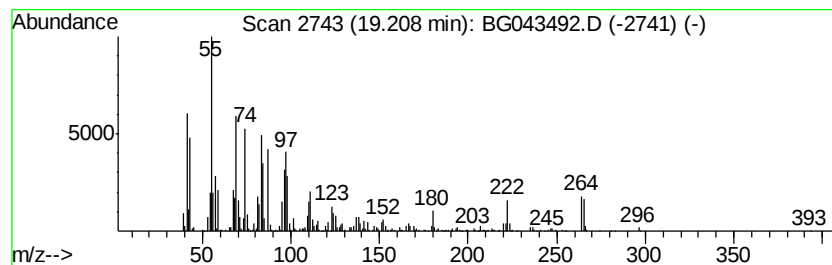
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.21	49.95 ng	1644440	Phenanthrene-d10	17.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	97
3		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	97
4		6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	95
5		cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
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Acq On : 4 Nov 2019 22:19
Operator : JU
Sample : K5676-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

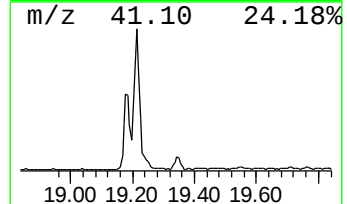
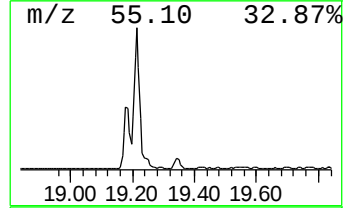
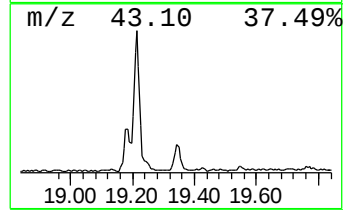
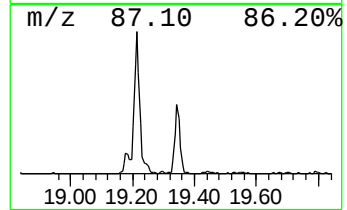
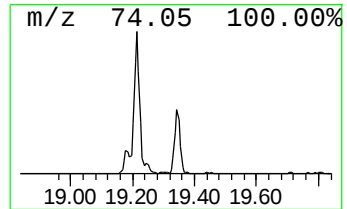
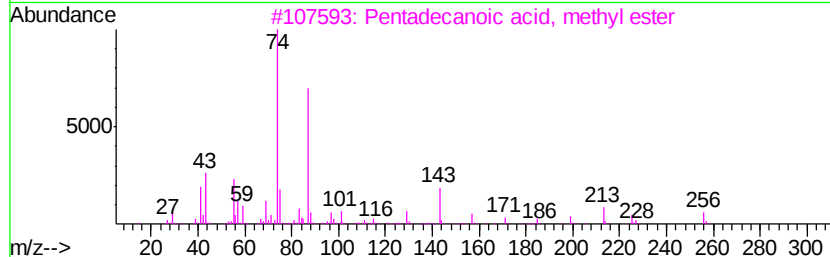
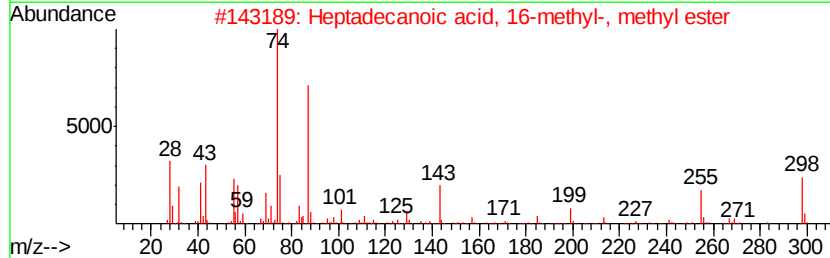
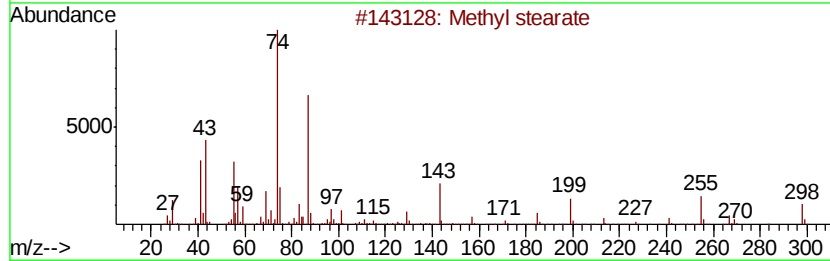
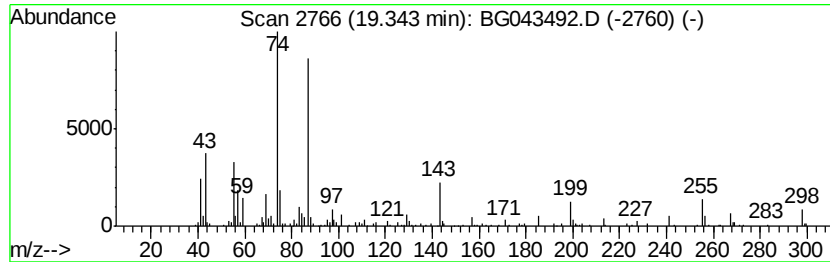
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	4.74 ng	156073	Phenanthrene-d10	17.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Methyl stearate	298 C19H38O2	000112-61-8 98
2		Heptadecanoic acid, 16-methyl-, ...	298 C19H38O2	005129-61-3 89
3		Pentadecanoic acid, methyl ester	256 C16H32O2	007132-64-1 83
4		Hexadecanoic acid, 15-methyl-, m...	284 C18H36O2	006929-04-0 72
5		Methyl 11-methyl-dodecanoate	228 C14H28O2	1000336-45-1 72



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110419\
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Sample : K5676-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

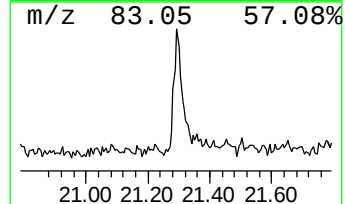
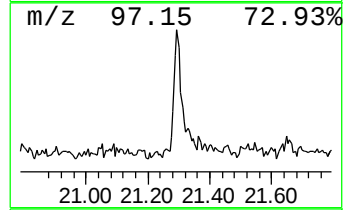
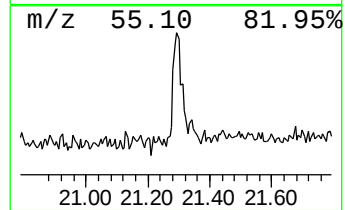
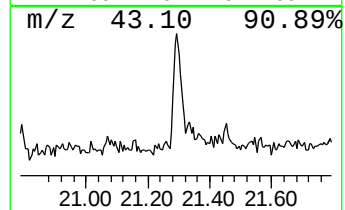
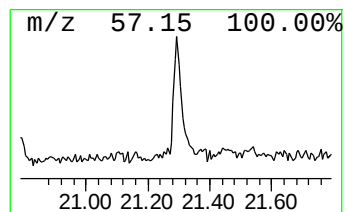
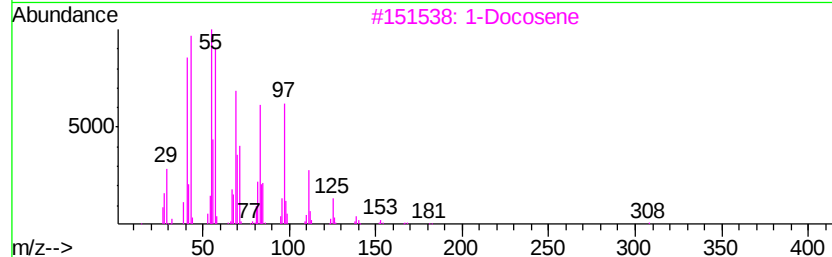
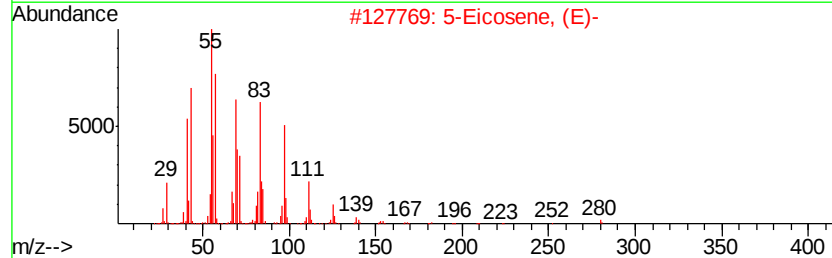
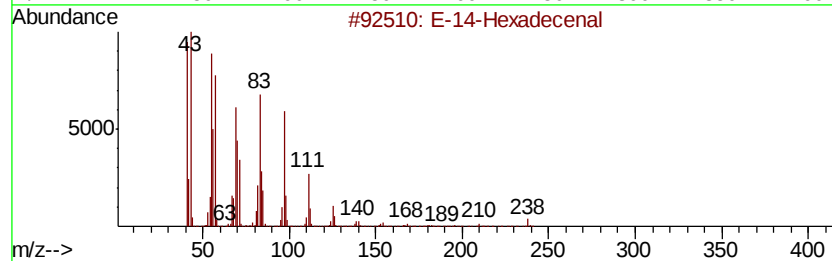
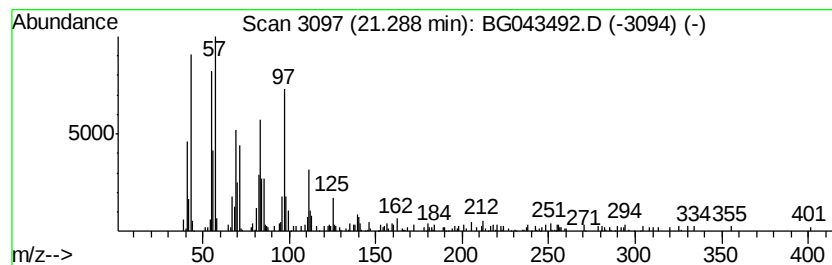
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 E-14-Hexadecenal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.29	4.11 ng	163915	Chrysene-d12	21.65	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	89
3	1-Docosene	308	C22H44	001599-67-3	87
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110419\
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Operator : JU
Sample : K5676-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.17	11.9	ng	131355	1	8.01	219812	20.0
2-Pentanone, 4-hy...	5.11	11.5	ng	126170	1	8.01	219812	20.0
unknown7.55	7.55	68.8	ng	756330	1	8.01	219812	20.0
Pentadecanoic aci...	18.04	11.5	ng	379057	4	17.39	658460	20.0
n-Hexadecanoic acid	18.27	3.6	ng	119029	4	17.39	658460	20.0
9,12-Octadecadien...	19.18	29.4	ng	969556	4	17.39	658460	20.0
9-Octadecenoic ac...	19.21	50.0	ng	1644440	4	17.39	658460	20.0
Methyl stearate	19.34	4.7	ng	156073	4	17.39	658460	20.0
E-14-Hexadecenal	21.29	4.1	ng	163915	5	21.65	797008	20.0