

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
 Data File : BG040964.D
 Acq On : 31 May 2019 00:00
 Operator : HP/JU
 Sample : K3090-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-4-D

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-BG052919.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	3.126	3	6	15	rVB2	118788	218123	3.71%	0.675%
2	3.209	15	20	35	rVB	416610	623654	10.61%	1.930%
3	5.653	429	436	449	rBV	1313597	2139012	36.39%	6.618%
4	7.269	701	711	722	rBV	1450650	2511651	42.73%	7.771%
5	7.651	767	776	784	rBV	1339853	2322856	39.52%	7.187%
6	8.121	850	856	868	rVB	258513	429656	7.31%	1.329%
7	8.444	904	911	919	rBV	984906	1673922	28.48%	5.179%
8	9.302	1048	1057	1067	rBV	835293	1533587	26.09%	4.745%
9	10.947	1330	1337	1345	rBV	311941	566018	9.63%	1.751%
10	13.373	1743	1750	1760	rBV	2343450	3637521	61.89%	11.255%
11	14.190	1883	1889	1895	rBV	270736	401787	6.84%	1.243%
12	14.754	1978	1985	1994	rVB3	538482	880206	14.98%	2.723%
13	16.241	2230	2238	2255	rBV	2204550	3325014	56.57%	10.288%
14	17.498	2444	2452	2463	rBV2	778726	1189587	20.24%	3.681%
15	18.350	2590	2597	2608	rBV	375090	567731	9.66%	1.757%
16	19.613	2808	2812	2822	rBV2	139313	211034	3.59%	0.653%
17	20.095	2887	2894	2900	rBV	4399178	5877427	100.00%	18.186%
18	21.370	3106	3111	3123	rBV2	250220	436445	7.43%	1.350%
19	21.775	3173	3180	3187	rBV2	810122	1340131	22.80%	4.147%
20	21.928	3202	3206	3213	rVB2	44832	66595	1.13%	0.206%
21	22.545	3305	3311	3320	rBV2	65604	135828	2.31%	0.420%
22	23.262	3426	3433	3444	rBV	82219	172820	2.94%	0.535%
23	24.084	3567	3573	3583	rVB2	75957	176797	3.01%	0.547%
24	25.118	3734	3749	3758	rBV2	412283	1407292	23.94%	4.354%
25	26.241	3932	3940	3951	rVB6	51125	154468	2.63%	0.478%
26	27.234	4100	4109	4121	rVB7	37771	147964	2.52%	0.458%
27	29.243	4439	4451	4453	rBV6	32030	100035	1.70%	0.310%
28	31.781	4873	4883	4884	rBV9	32676	71788	1.22%	0.222%

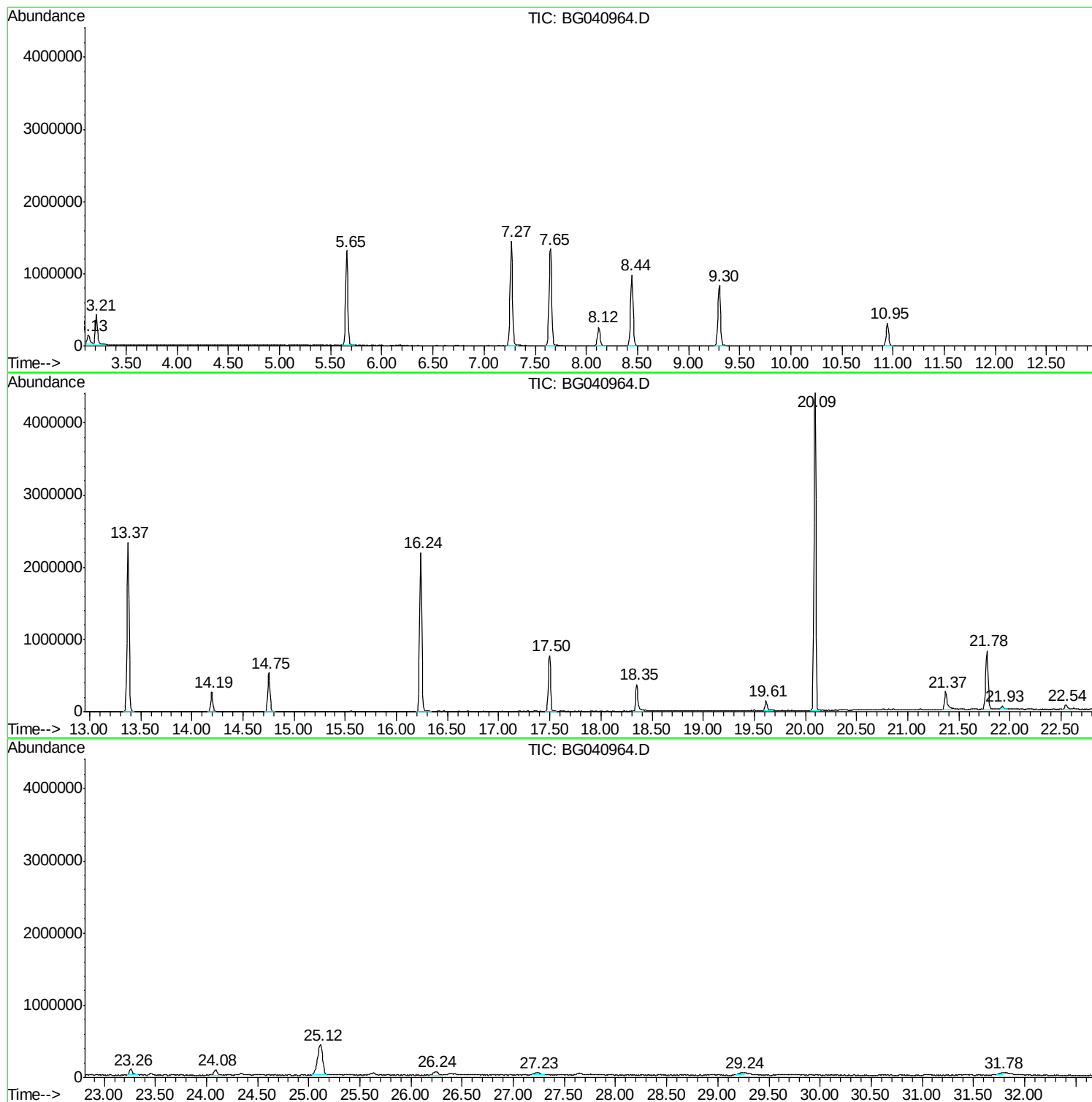
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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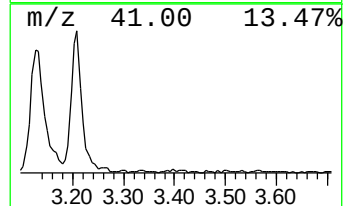
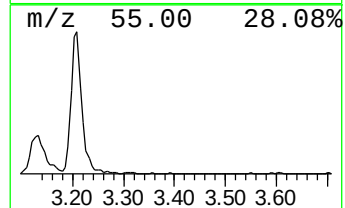
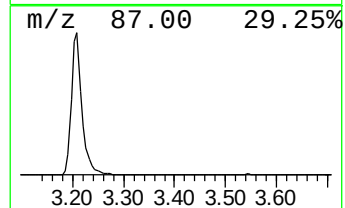
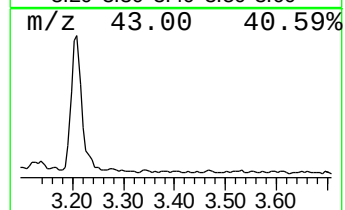
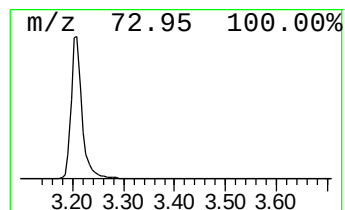
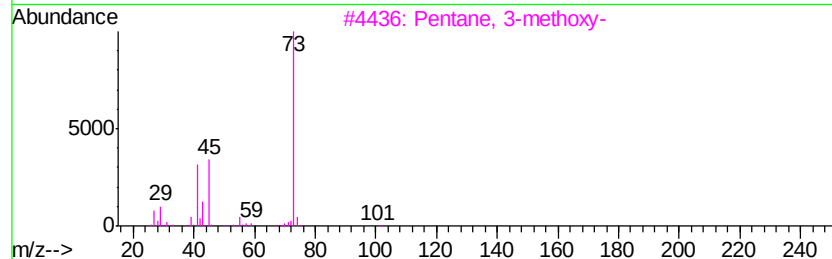
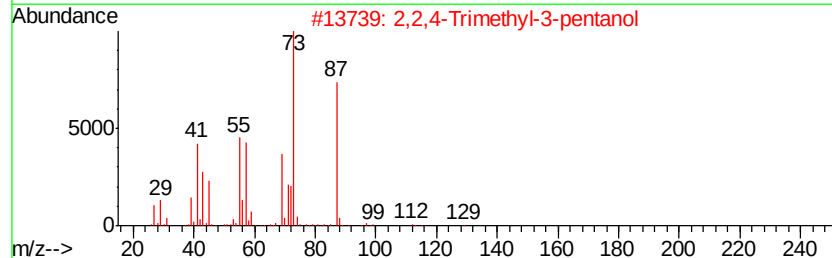
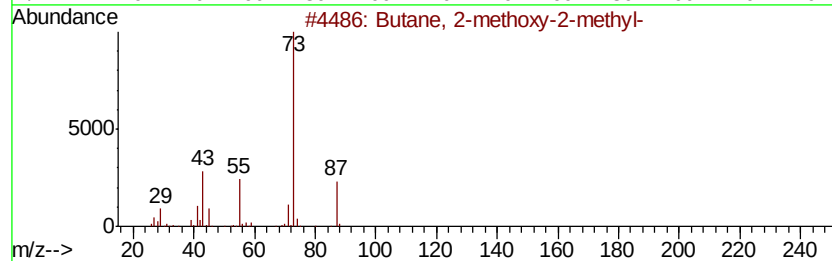
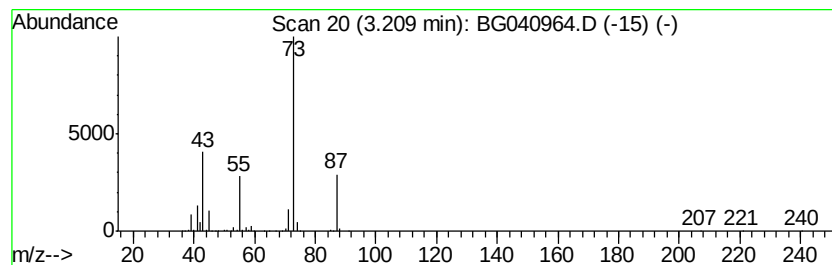
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	29.03 ng	623654	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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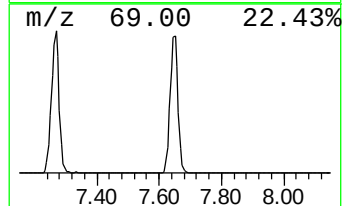
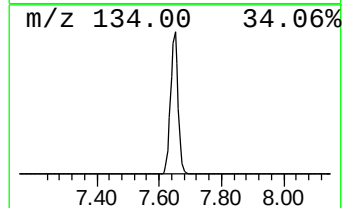
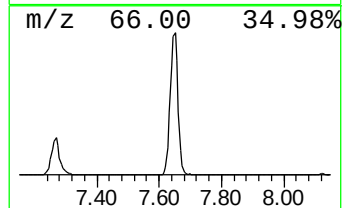
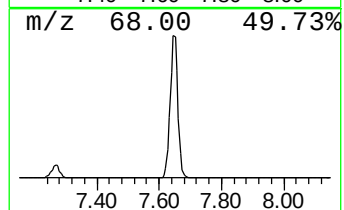
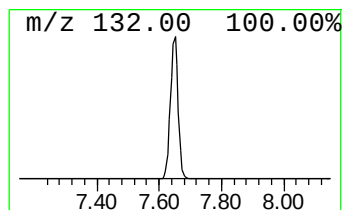
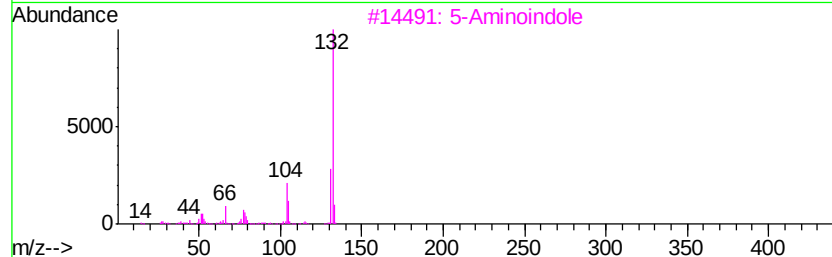
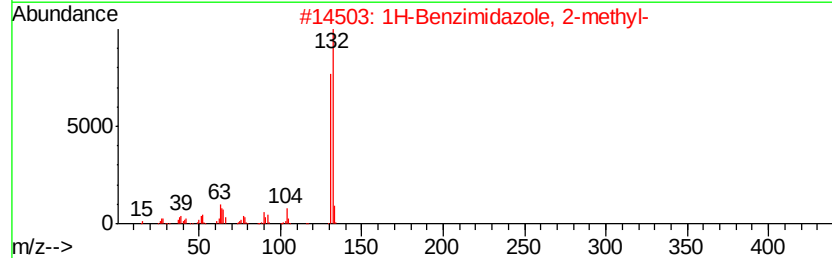
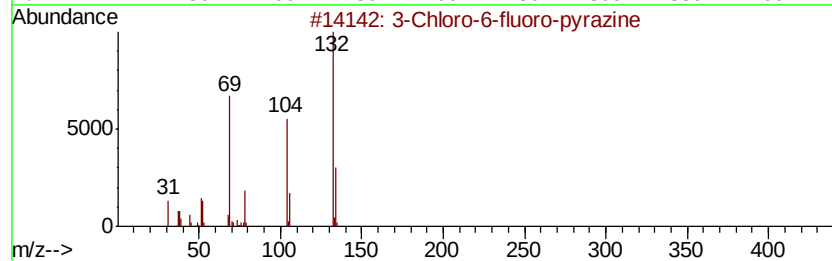
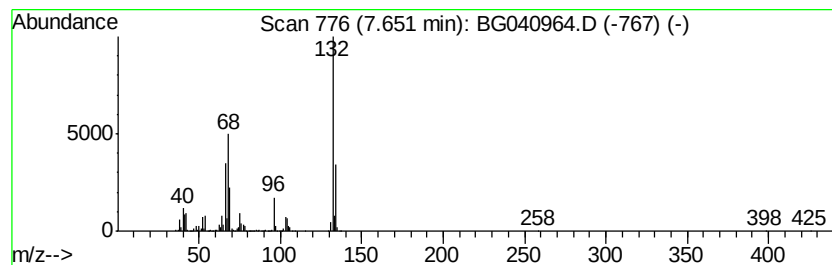
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	108.13 ng	2322860	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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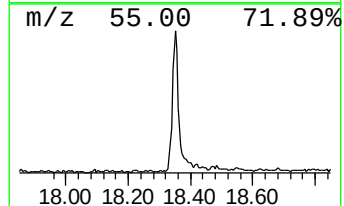
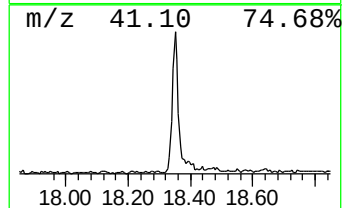
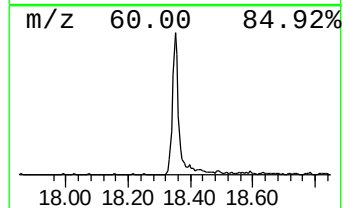
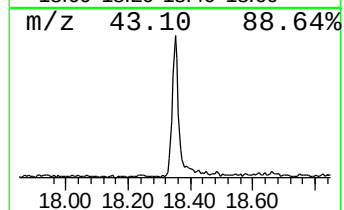
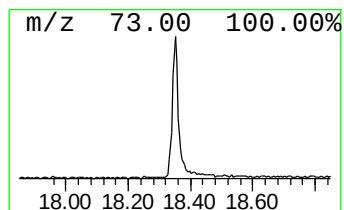
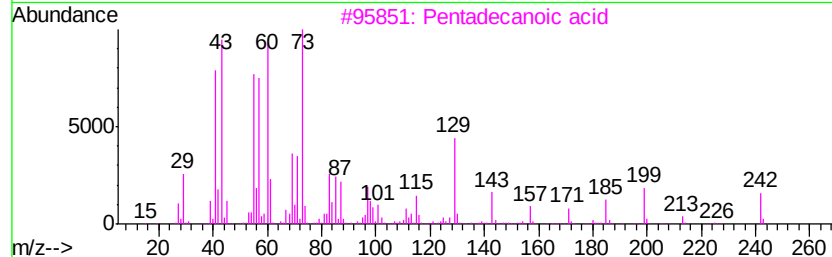
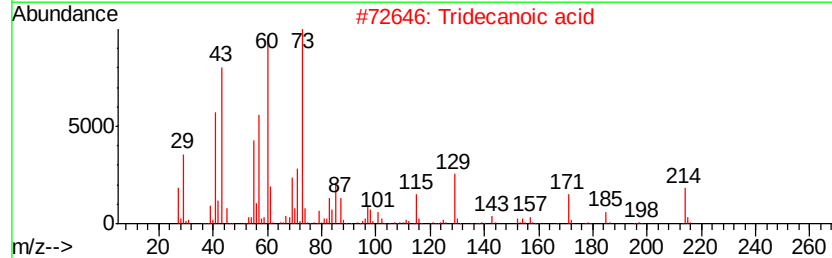
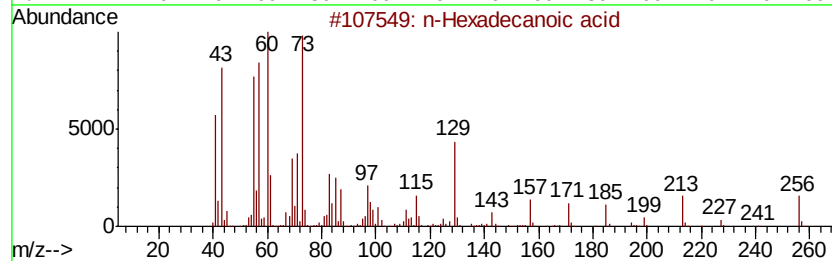
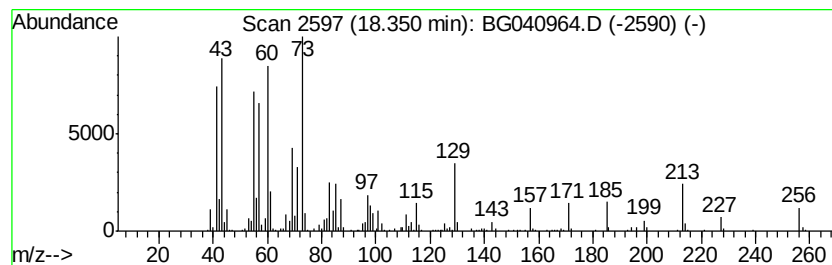
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	9.55 ng	567731	Phenanthrene-d10	17.50

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62



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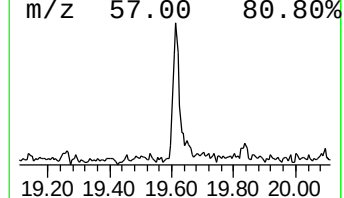
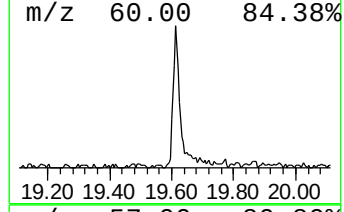
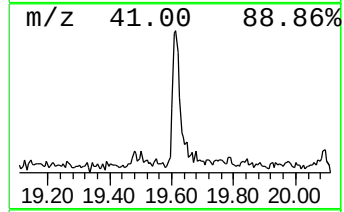
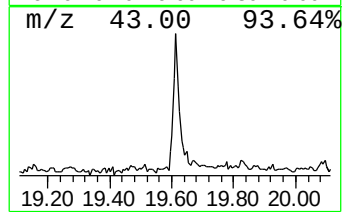
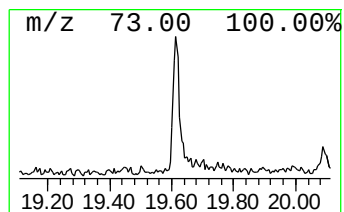
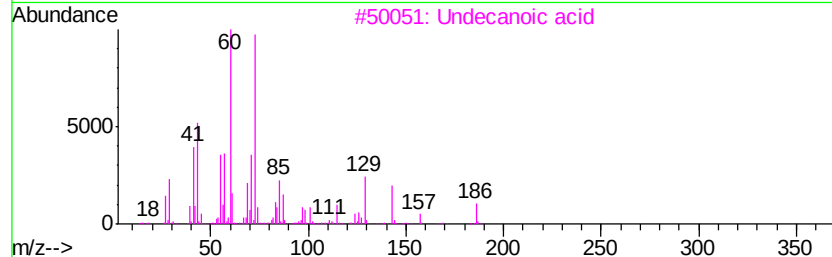
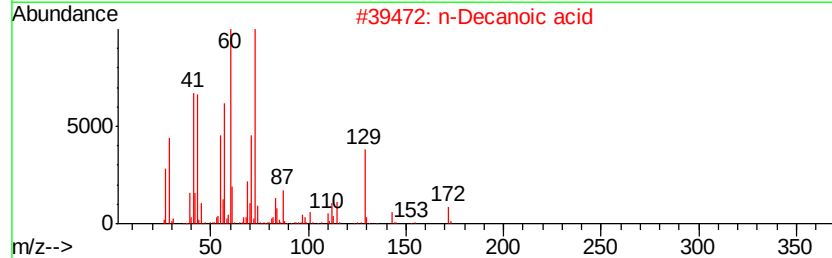
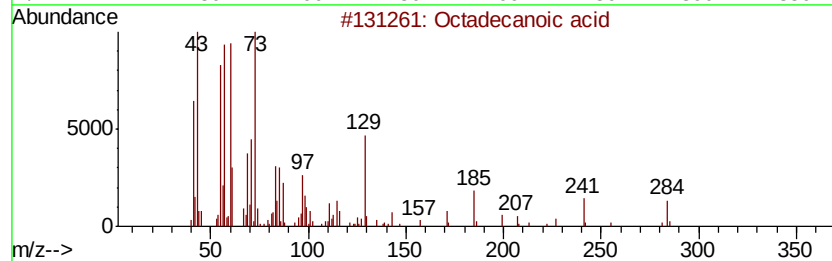
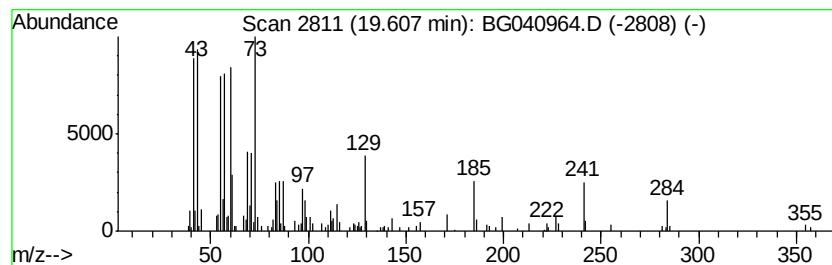
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Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	3.55 ng	211034	Phenanthrene-d10	17.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	n-Decanoic acid	172	C10H20O2	000334-48-5	60
3	Undecanoic acid	186	C11H22O2	000112-37-8	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	52
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	30



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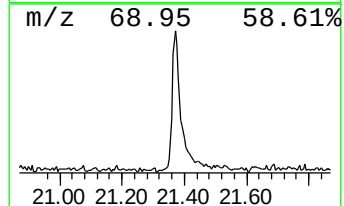
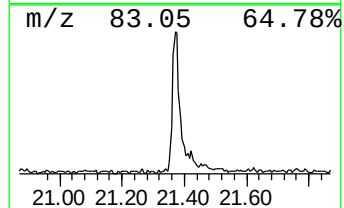
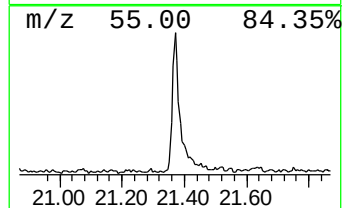
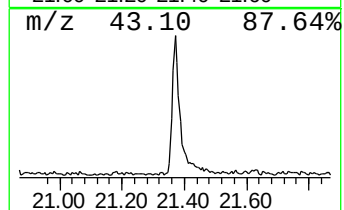
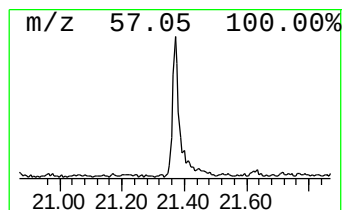
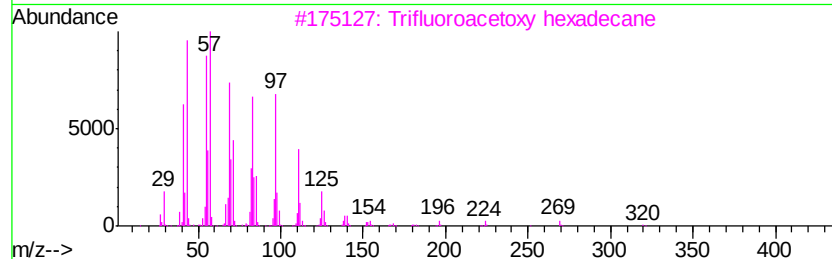
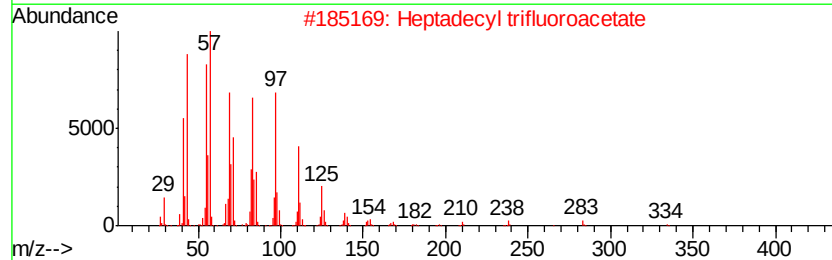
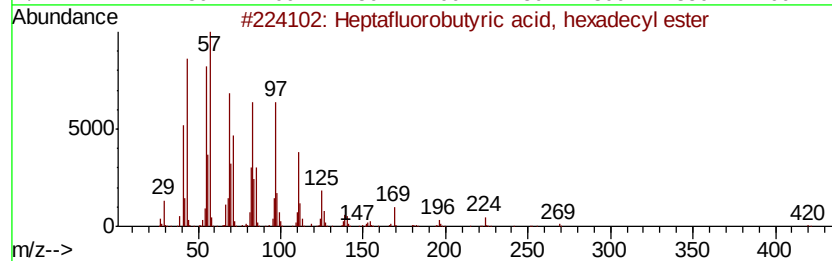
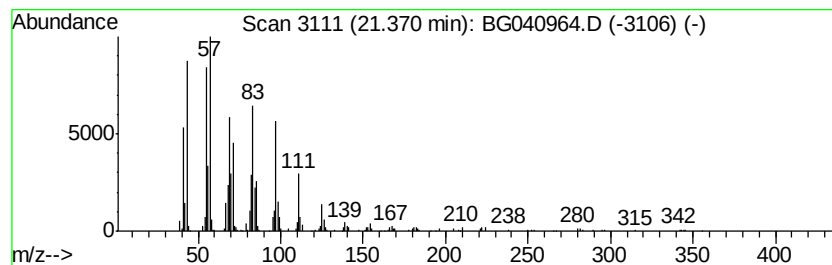
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Heptafluorobutyric acid, he... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	6.51 ng	436445	Chrysene-d12	21.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	94
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	93



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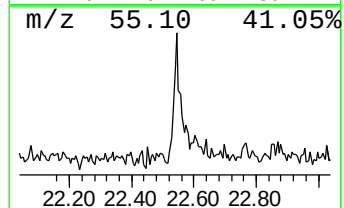
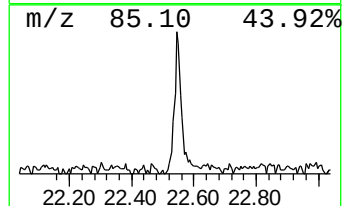
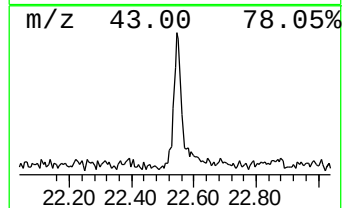
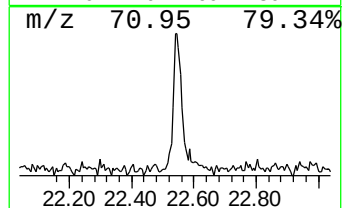
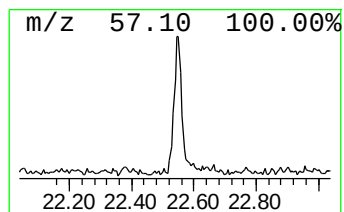
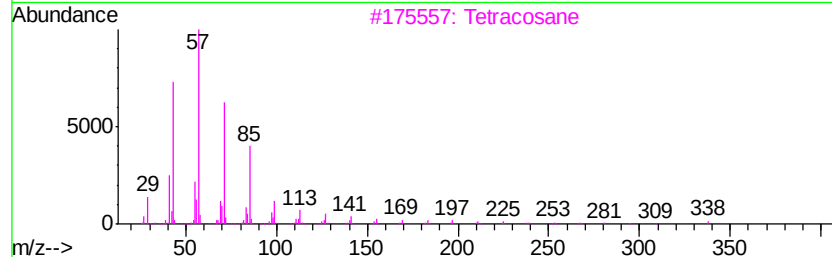
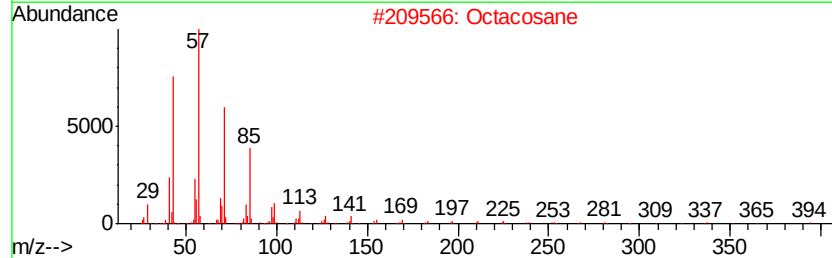
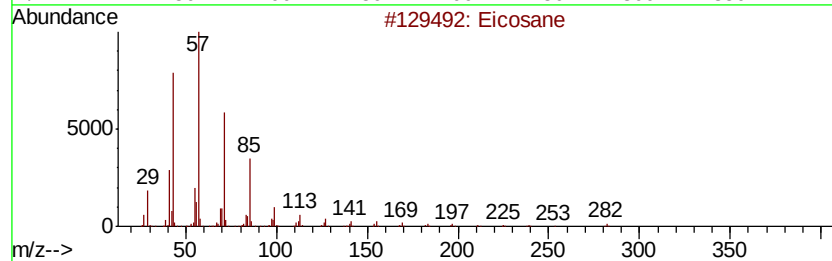
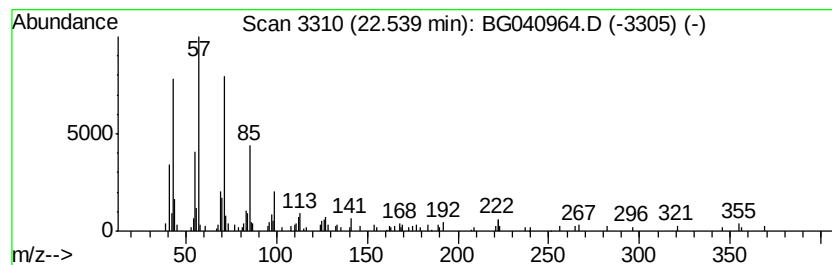
Instrument :
BNA_G
ClientSampleId :
TP-4-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.54	2.03 ng	135828	Chrysene-d12	21.78
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 92
2	Octacosane		394 C28H58	000630-02-4 90
3	Tetracosane		338 C24H50	000646-31-1 87
4	Heneicosane		296 C21H44	000629-94-7 87
5	Octadecane		254 C18H38	000593-45-3 86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040964.D
Acq On : 31 May 2019 00:00
Operator : HP/JU
Sample : K3090-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

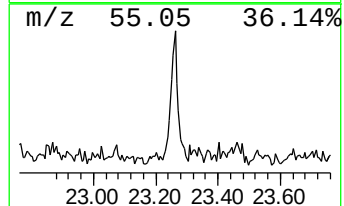
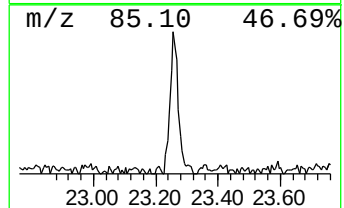
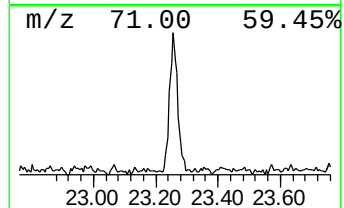
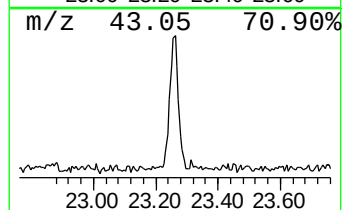
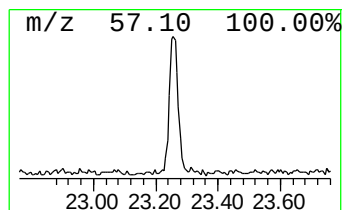
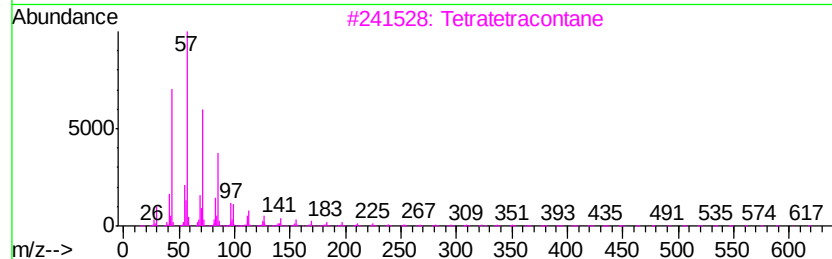
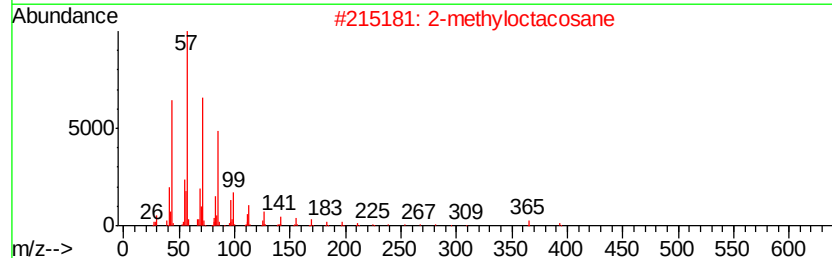
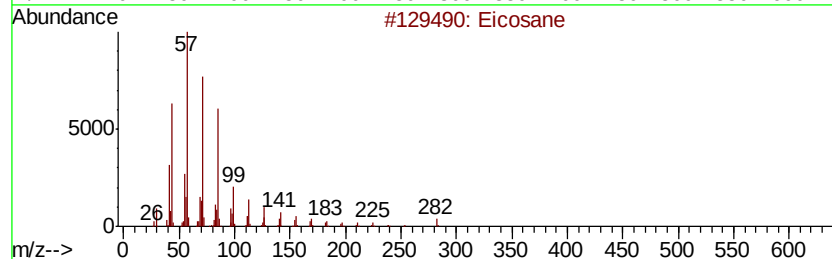
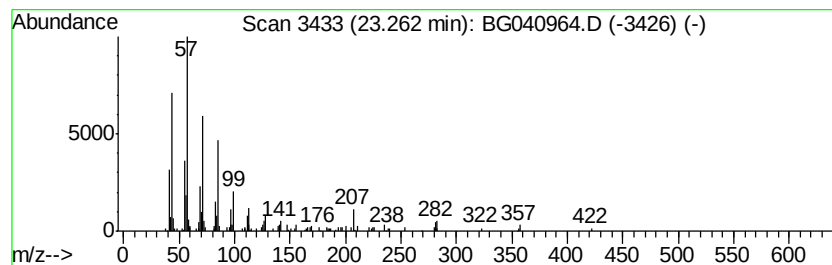
Instrument :
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ClientSampleId :
TP-4-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.26	2.58 ng	172820	Chrysene-d12	21.78
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	91
2	2-methyloctacosane	408 C29H60	1000376-72-8	81
3	Tetratetracontane	619 C44H90	007098-22-8	76
4	Dodecane, 2-methyl-	184 C13H28	001560-97-0	76
5	triacontane	422 C30H62	000638-68-6	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040964.D
Acq On : 31 May 2019 00:00
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Sample : K3090-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-D

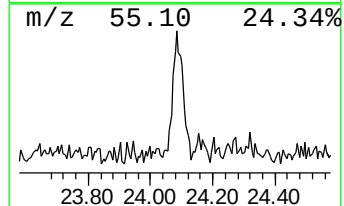
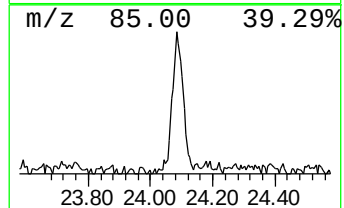
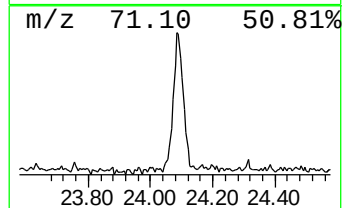
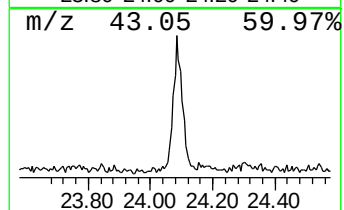
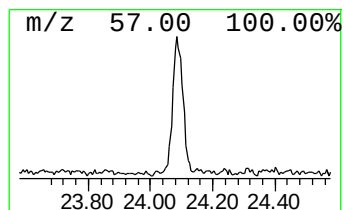
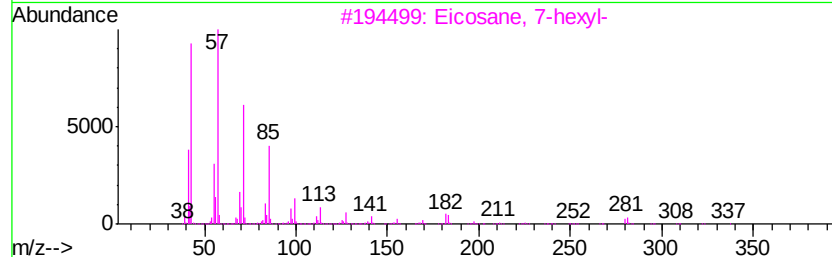
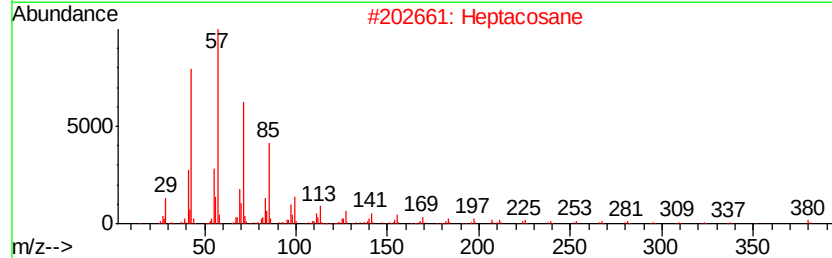
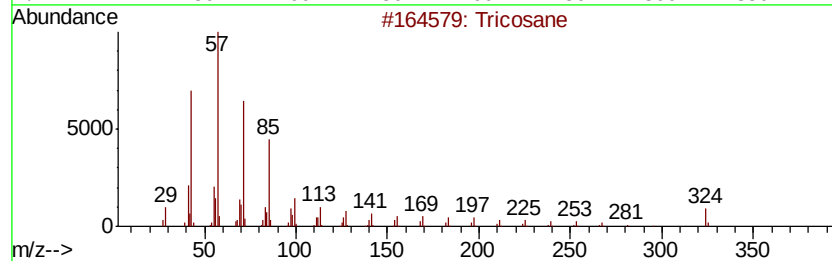
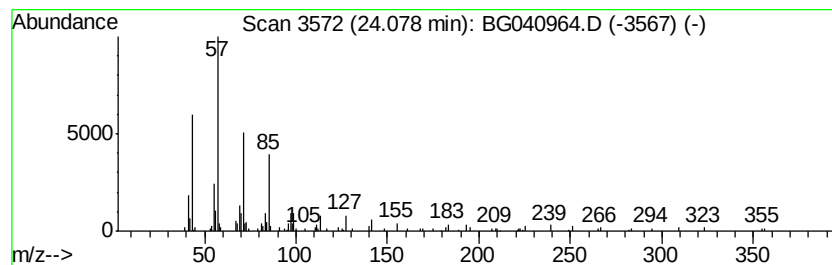
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tricosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.08	2.51 ng	176797	Perylene-d12	25.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
Data File : BG040964.D
Acq On : 31 May 2019 00:00
Operator : HP/JU
Sample : K3090-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-D

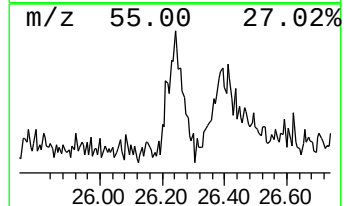
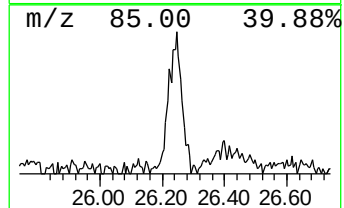
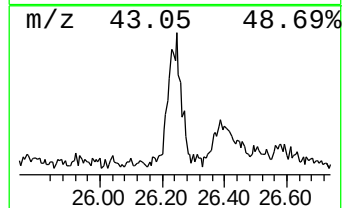
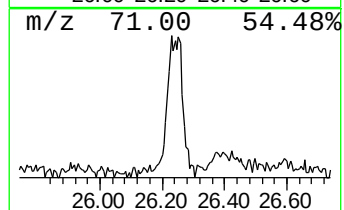
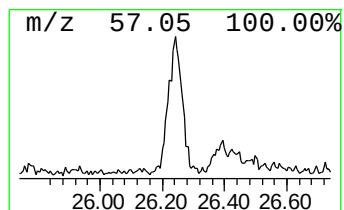
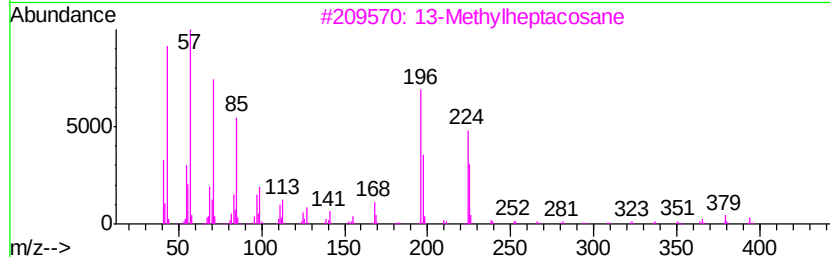
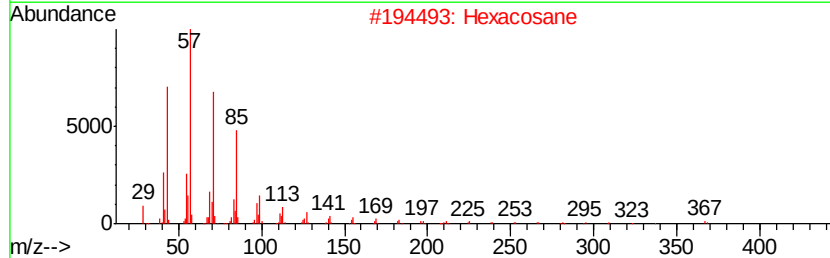
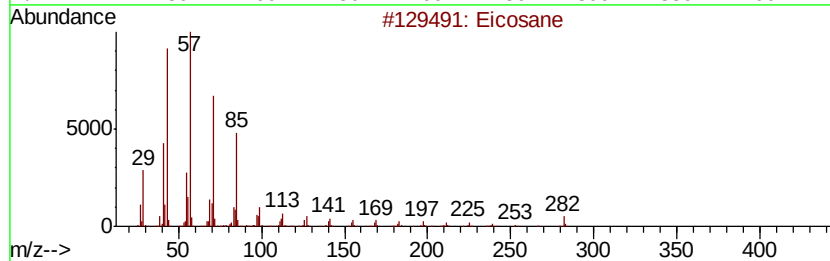
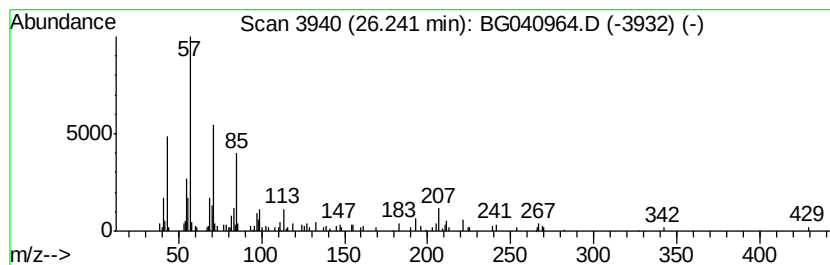
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 13-Methylheptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.24	2.20 ng	154468	Perylene-d12	25.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	80
2		Hexacosane	366	C26H54	000630-01-3	80
3		13-Methylheptacosane	394	C28H58	015689-72-2	74
4		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	72
5		Tetracosane	338	C24H50	000646-31-1	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG053019\
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Acq On : 31 May 2019 00:00
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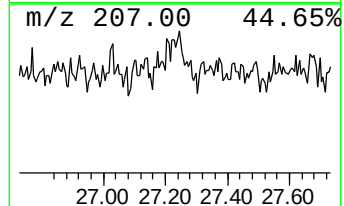
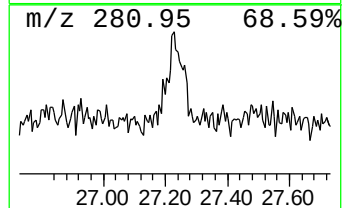
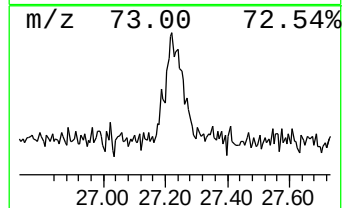
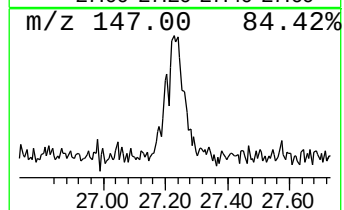
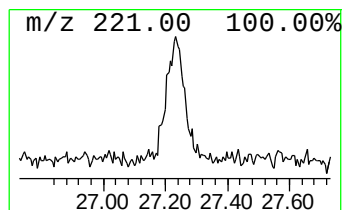
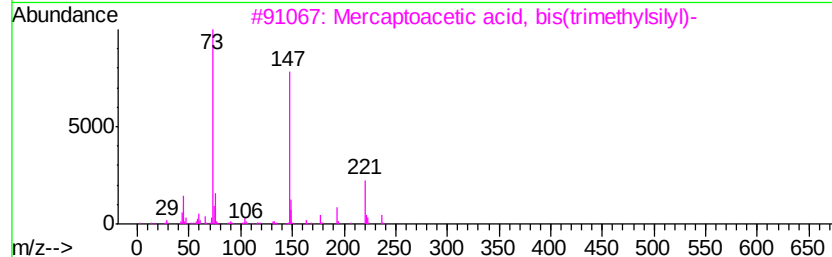
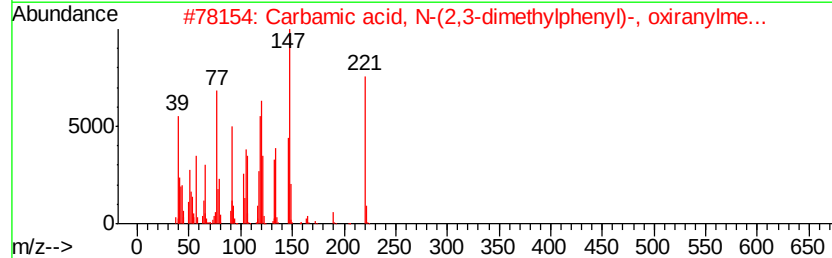
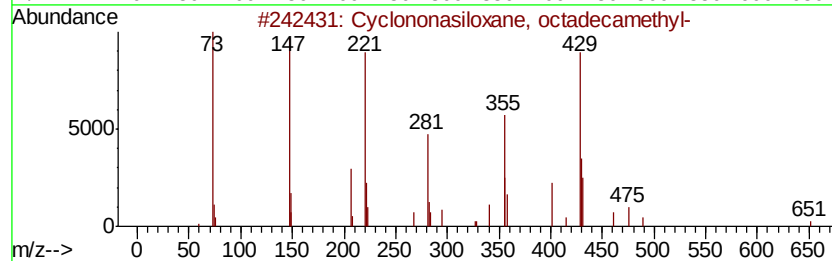
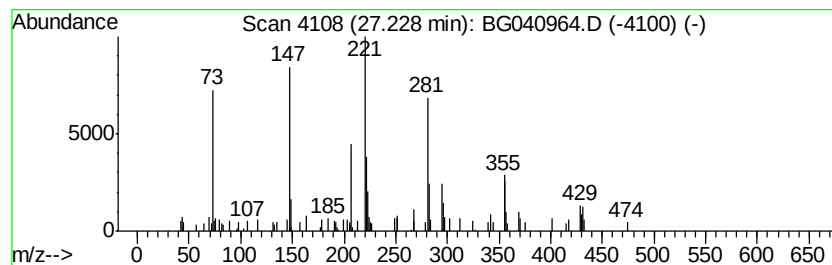
Instrument :
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ClientSampleId :
TP-4-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG052919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclononasiloxane, octadeca... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
27.23	2.10 ng	147964	Perylene-d12	25.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
2		Carbamic acid, N-(2,3-dimethylph...	221	C12H15NO3	339273-79-9	43
3		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	37
4		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	27
5		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG053019\
Data File : BG040964.D
Acq On : 31 May 2019 00:00
Operator : HP/JU
Sample : K3090-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG052919.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...	3.21	29.0	ng	623654	1	8.12	429656	20.0
unknown7.65	7.65	108.1	ng	2322860	1	8.12	429656	20.0
n-Hexadecanoic acid	18.35	9.6	ng	567731	4	17.50	1189590	20.0
Octadecanoic acid	19.61	3.5	ng	211034	4	17.50	1189590	20.0
Heptafluorobutyri...	21.37	6.5	ng	436445	5	21.78	1340130	20.0
Eicosane	22.54	2.0	ng	135828	5	21.78	1340130	20.0
2-methyloctacosane	23.26	2.6	ng	172820	5	21.78	1340130	20.0
Tricosane	24.08	2.5	ng	176797	6	25.12	1407290	20.0
13-Methylheptacosane	26.24	2.2	ng	154468	6	25.12	1407290	20.0
Cyclononasiloxane...	27.23	2.1	ng	147964	6	25.12	1407290	20.0