

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
 Data File : BG043826.D
 Acq On : 17 Dec 2019 19:20
 Operator : JU
 Sample : K6294-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-1

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-BG120919.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	3.123	3	6	14	rVB	56426	92394	1.07%	0.194%
2	3.200	14	19	29	rVB	227950	337866	3.90%	0.711%
3	5.115	338	345	353	rBV	393877	626109	7.22%	1.318%
4	5.579	417	424	438	rBV	1794100	2879545	33.22%	6.060%
5	7.166	685	694	707	rBV	2056514	3619137	41.75%	7.617%
6	7.536	749	757	766	rBV	1896529	3279589	37.83%	6.902%
7	8.000	828	836	845	rBV	369055	624320	7.20%	1.314%
8	8.323	883	891	899	rBV	1330449	2397860	27.66%	5.047%
9	9.151	1022	1032	1043	rBV	1128977	2080981	24.01%	4.380%
10	10.802	1305	1313	1322	rBV	543628	975305	11.25%	2.053%
11	13.253	1723	1730	1742	rBV	3340626	5298642	61.13%	11.152%
12	14.075	1864	1870	1881	rBV	213648	320369	3.70%	0.674%
13	14.627	1956	1964	1972	rBV	1021102	1626741	18.77%	3.424%
14	16.114	2209	2217	2230	rBV	3094538	4698514	54.20%	9.889%
15	17.371	2424	2431	2442	rBV	1395453	2139544	24.68%	4.503%
16	19.986	2869	2876	2884	rBV	6177887	8668197	100.00%	18.243%
17	21.296	3094	3099	3108	rBV2	486767	818957	9.45%	1.724%
18	21.625	3148	3155	3166	rVV	1362323	2247513	25.93%	4.730%
19	21.854	3189	3194	3200	rBV	160473	226180	2.61%	0.476%
20	22.459	3292	3297	3309	rBV2	219498	464236	5.36%	0.977%
21	23.147	3409	3414	3425	rVB2	223946	438065	5.05%	0.922%
22	23.388	3451	3455	3464	rVB2	75284	160817	1.86%	0.338%
23	23.952	3545	3551	3563	rVB	208143	450836	5.20%	0.949%
24	24.463	3630	3638	3646	rBV4	90351	264650	3.05%	0.557%
25	24.786	3683	3693	3704	rBV2	632248	2015206	23.25%	4.241%
26	24.892	3706	3711	3721	rVB4	171631	452876	5.22%	0.953%
27	26.020	3896	3903	3914	rVB2	104356	310478	3.58%	0.653%

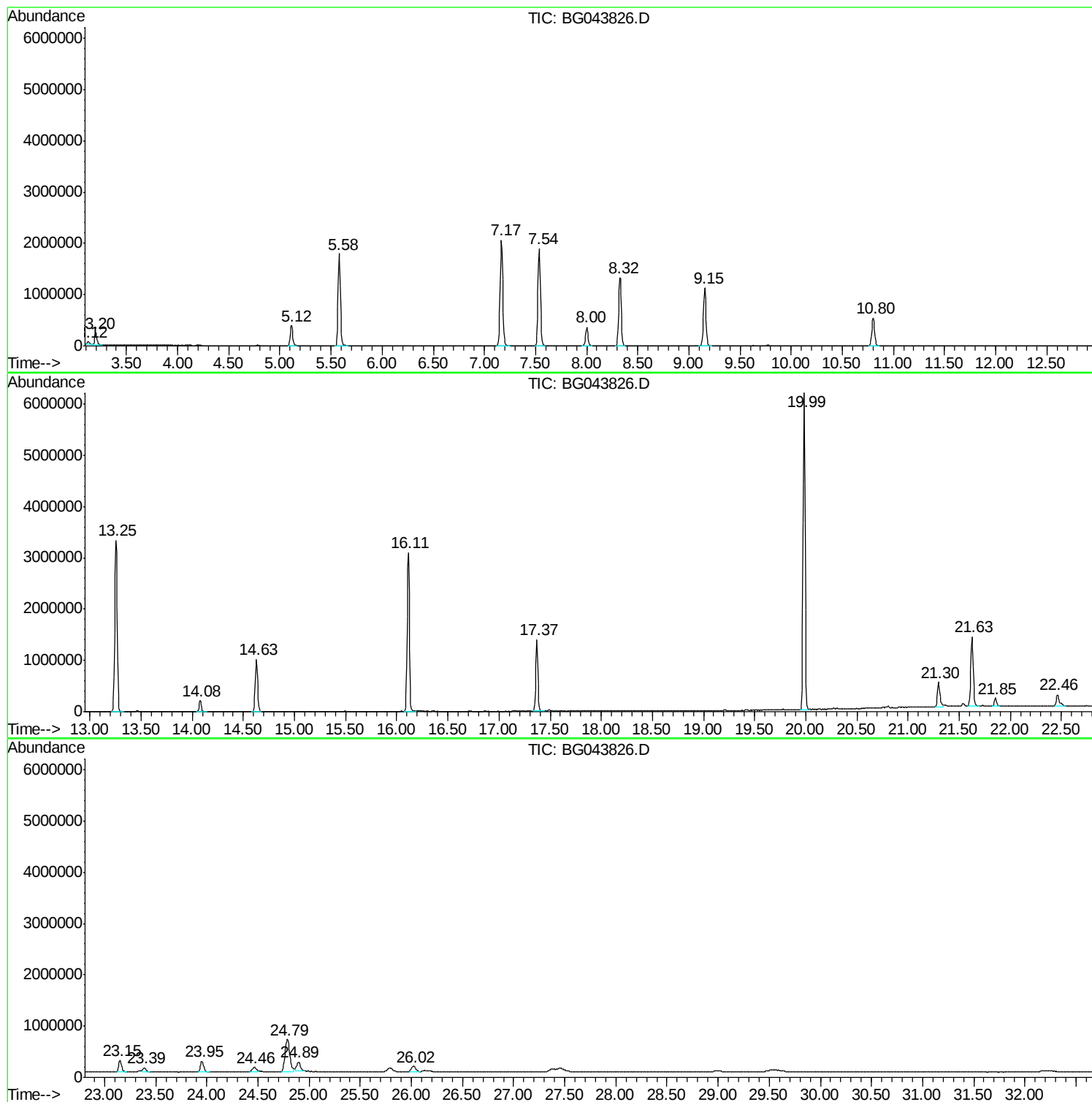
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG120919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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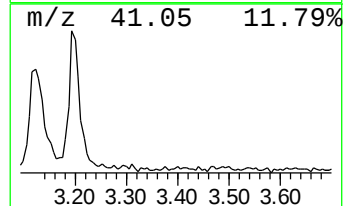
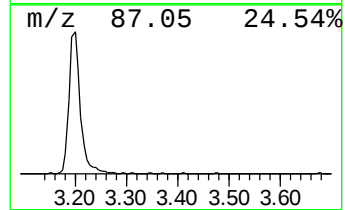
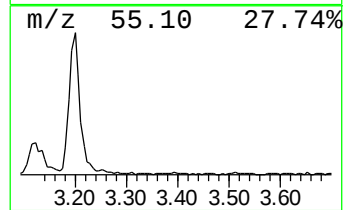
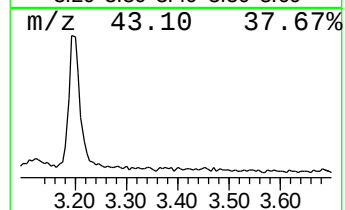
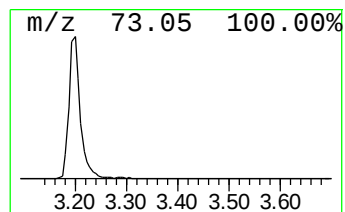
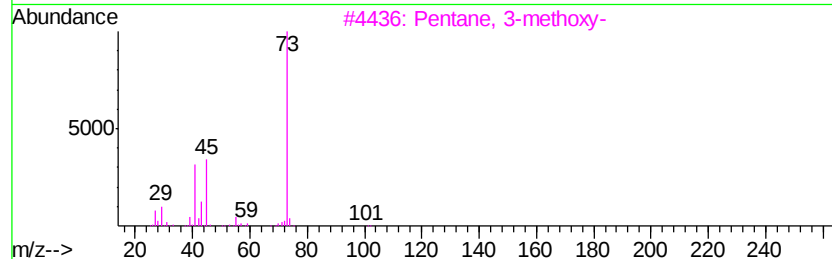
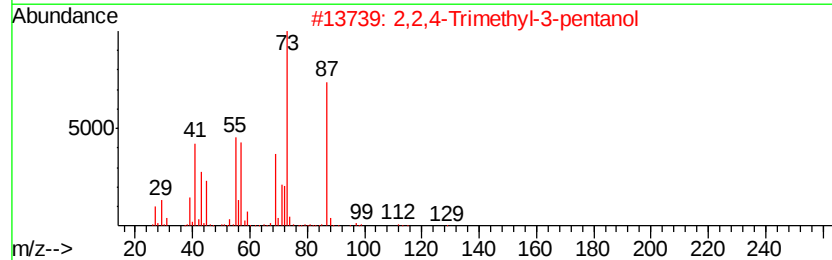
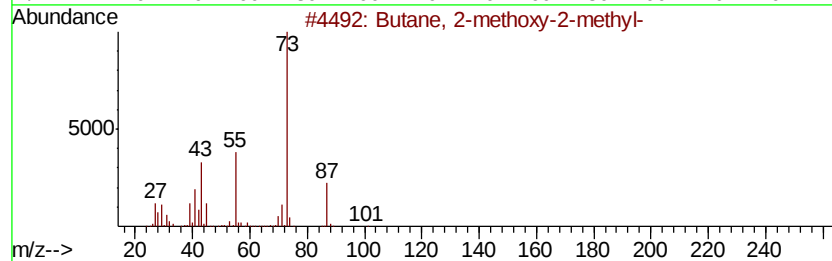
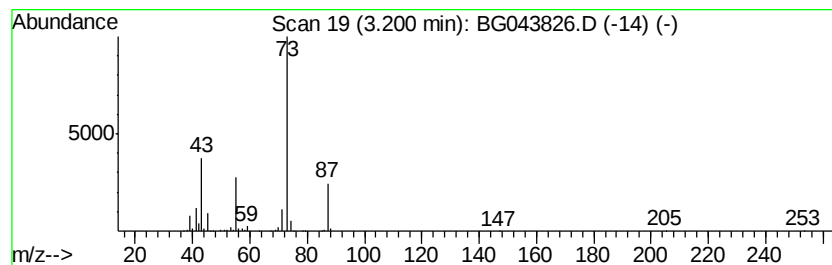
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	10.82 ng	337866	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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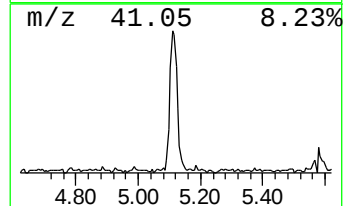
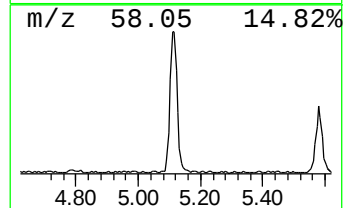
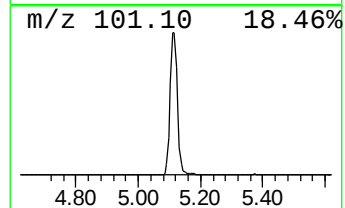
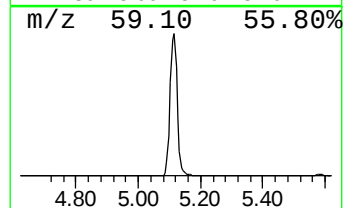
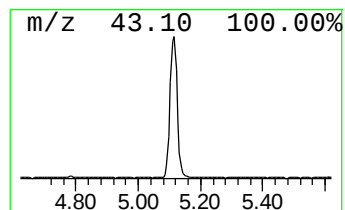
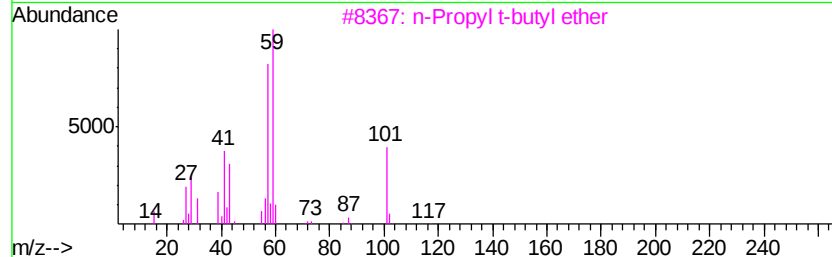
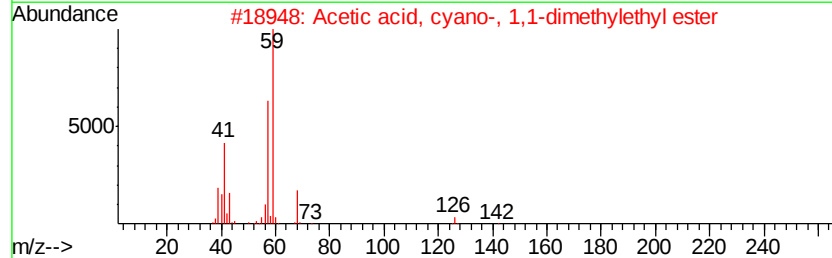
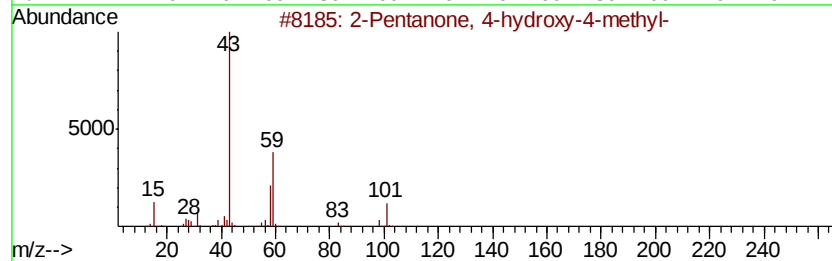
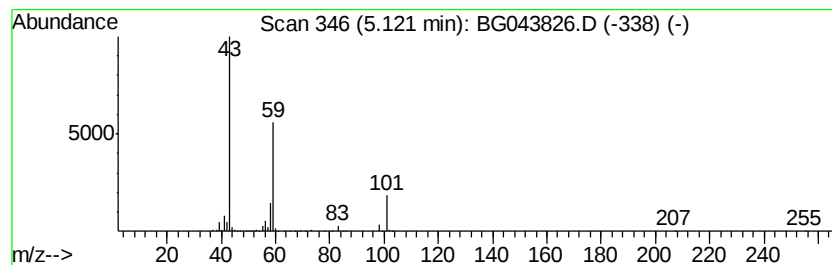
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	20.06 ng	626109	1,4-Dichlorobenzene-d4	8.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	37	
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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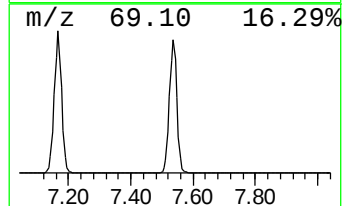
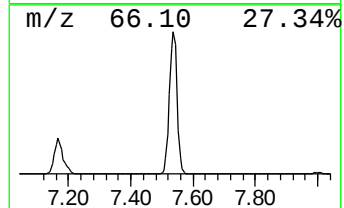
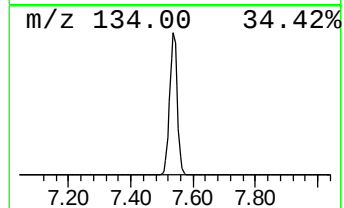
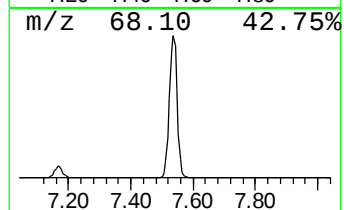
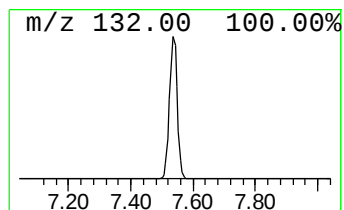
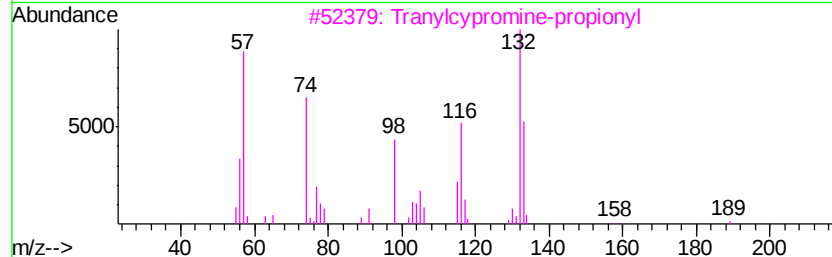
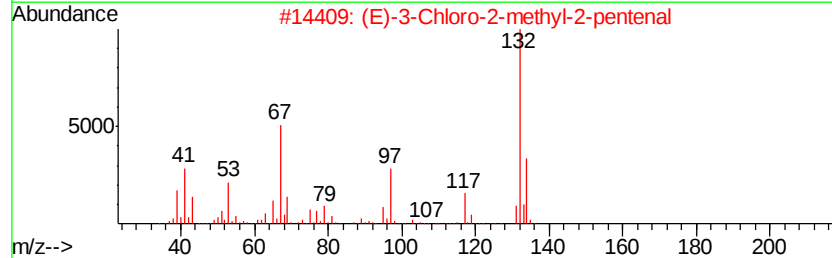
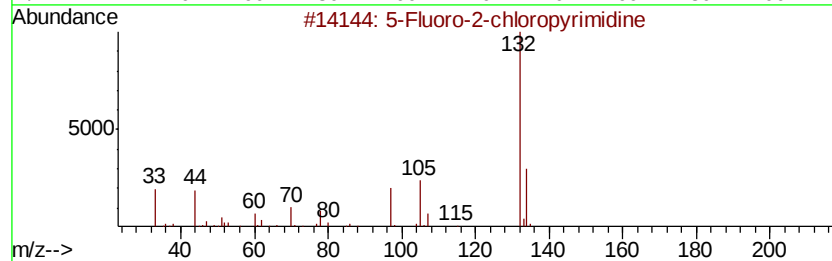
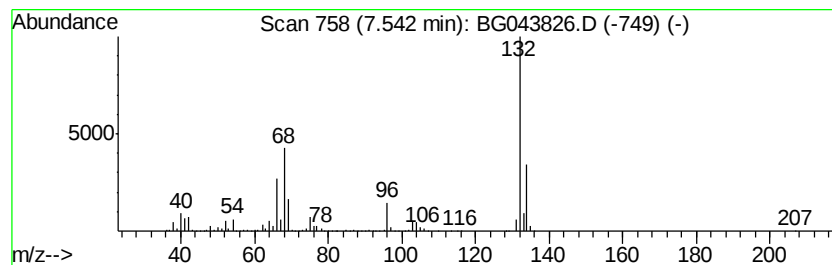
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Peak Number 4 unknown7.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	105.06 ng	3279590	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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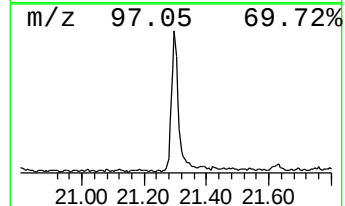
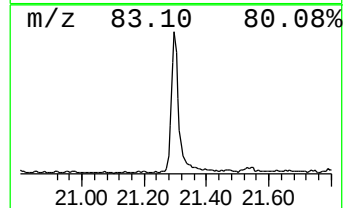
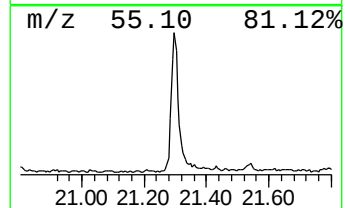
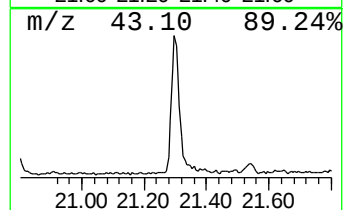
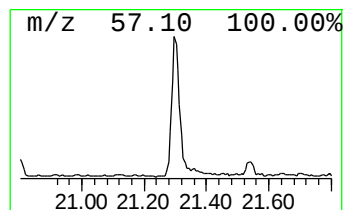
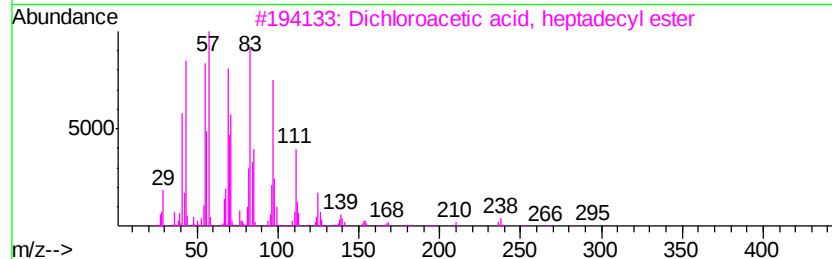
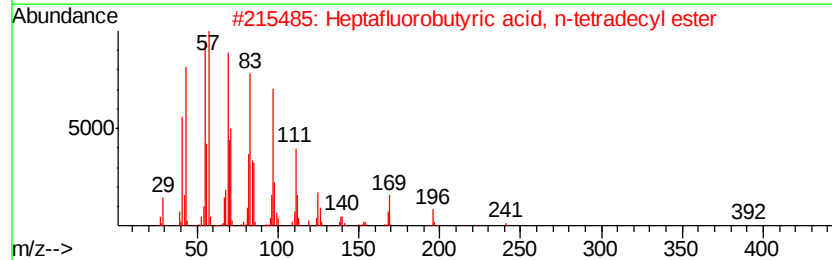
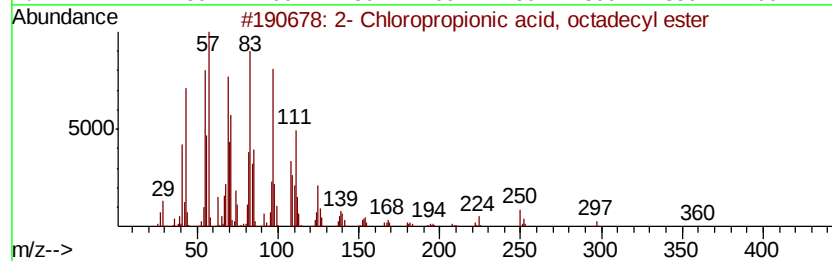
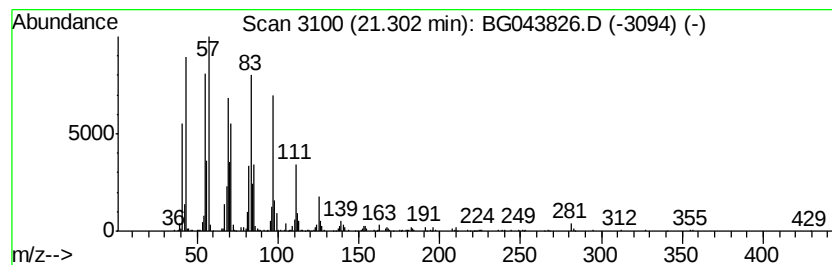
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Peak Number 6 2- Chloropropionic acid, oc... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.30	7.29 ng	818957	Chrysene-d12	21.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2	Heptafluorobutyric acid, n-tetra...		410	C18H29F7O2	007365-36-8	94
3	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	94
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
5	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	94



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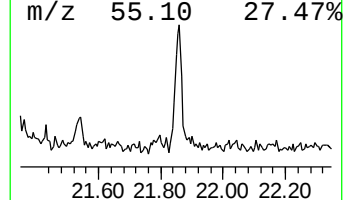
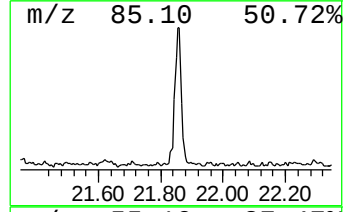
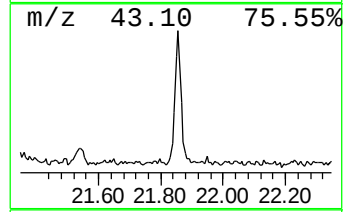
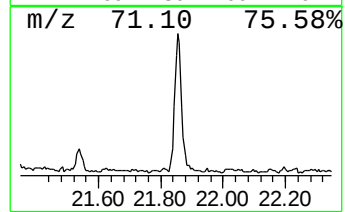
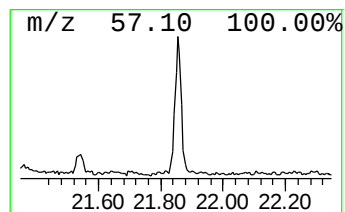
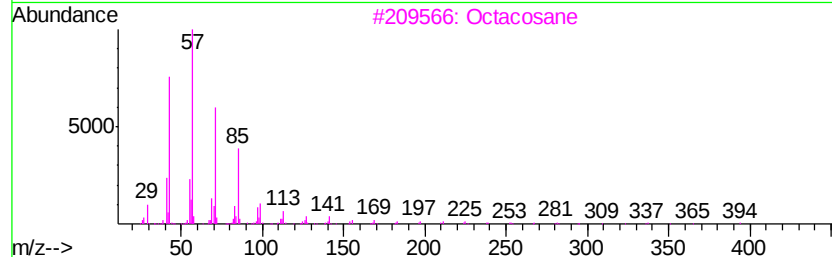
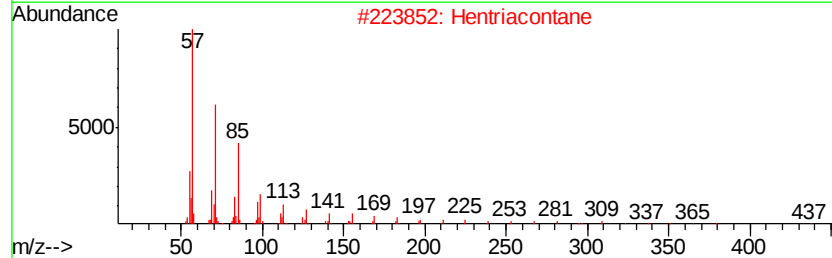
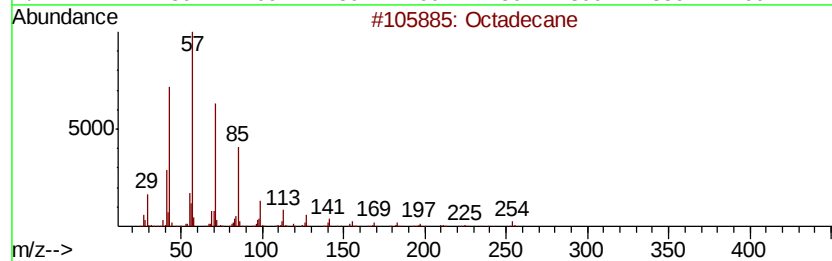
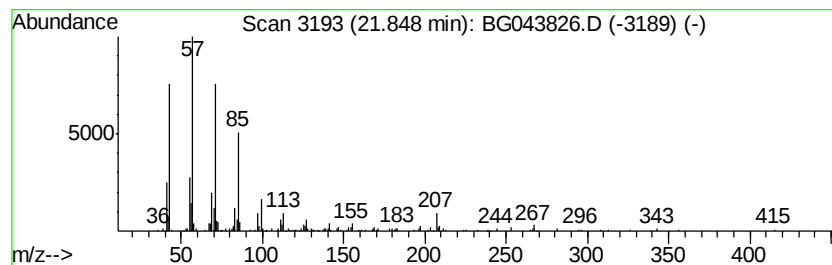
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 Peak Number 7 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.85	2.01 ng	226180	Chrysene-d12		21.63	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Tetracosane	338	C24H50	000646-31-1	90
5		Hexacosane	366	C26H54	000630-01-3	90



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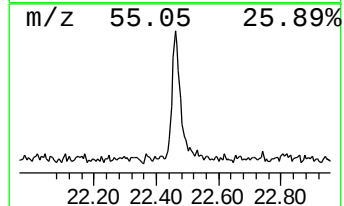
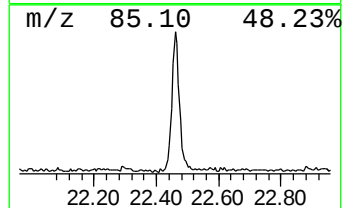
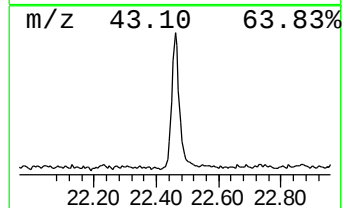
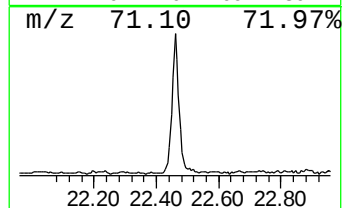
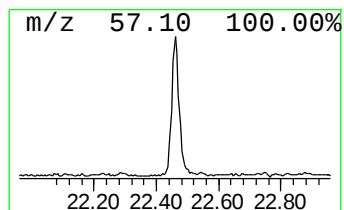
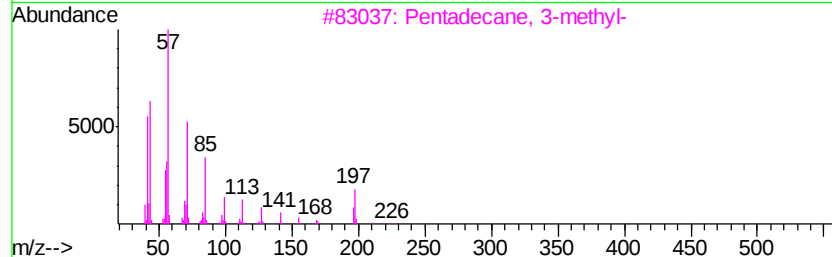
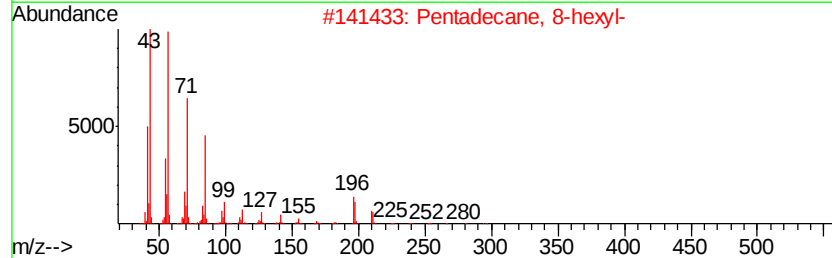
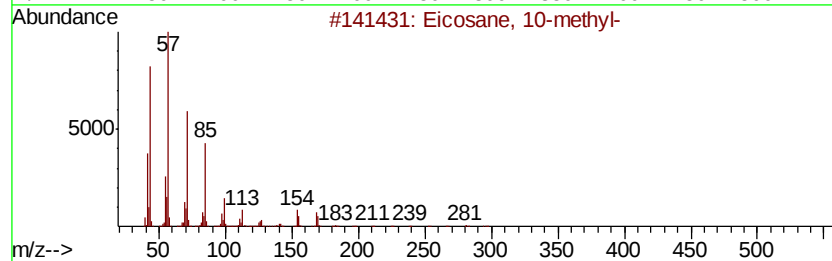
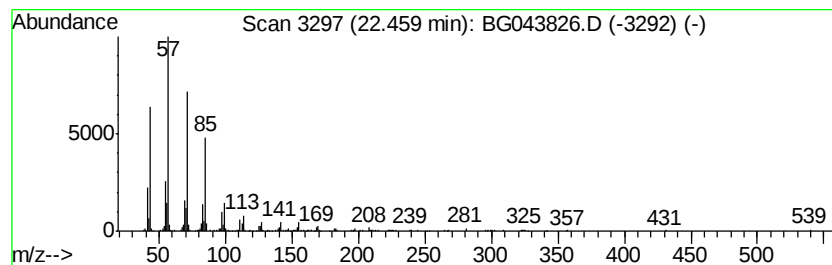
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane, 10-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.46	4.13 ng	464236	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
3		Pentadecane, 3-methyl-	226	C16H34	002882-96-4	90
4		Tricosane	324	C23H48	000638-67-5	89
5		Nonadecane	268	C19H40	000629-92-5	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043826.D
Acq On : 17 Dec 2019 19:20
Operator : JU
Sample : K6294-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-1

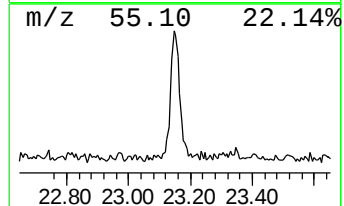
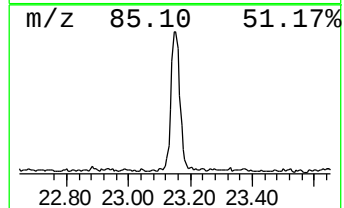
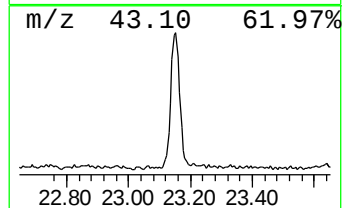
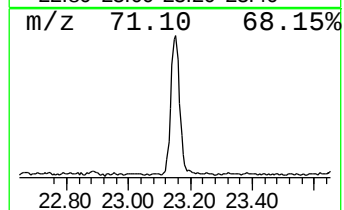
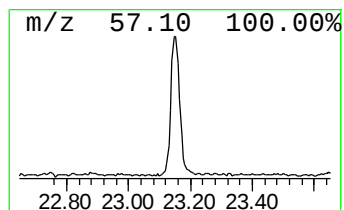
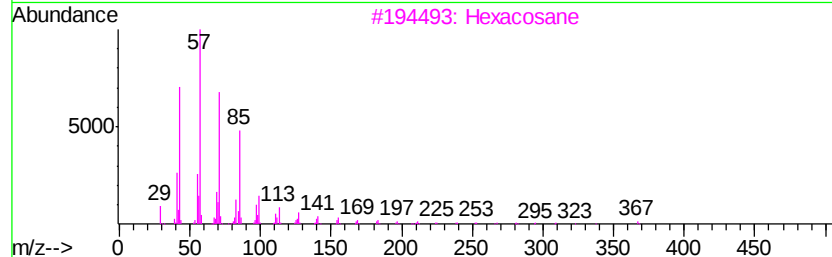
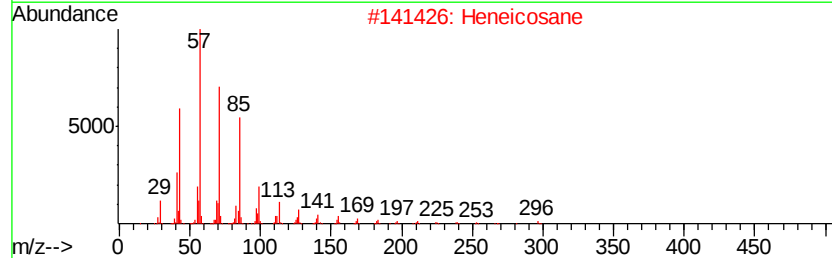
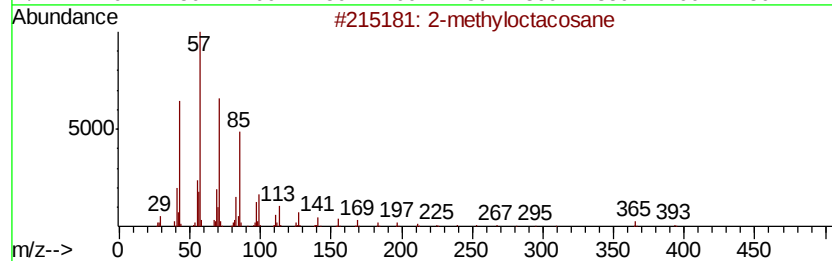
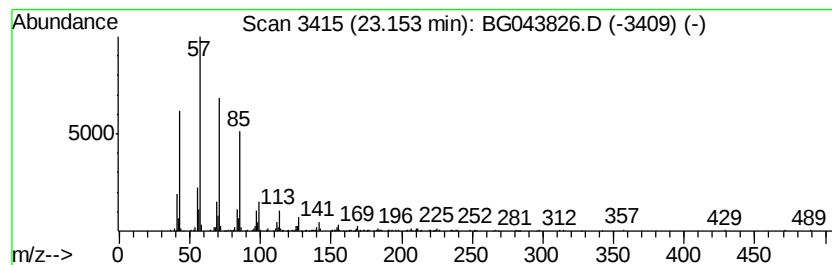
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	3.90 ng	438065	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043826.D
Acq On : 17 Dec 2019 19:20
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Sample : K6294-01
Misc :
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Instrument :
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ClientSampleId :
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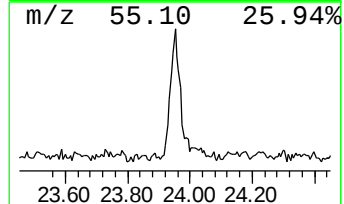
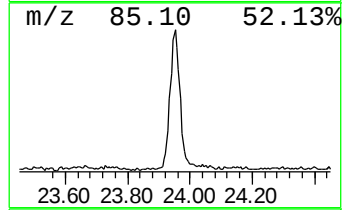
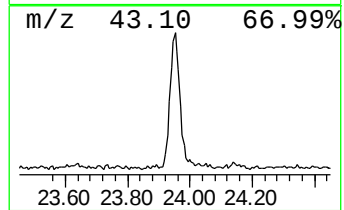
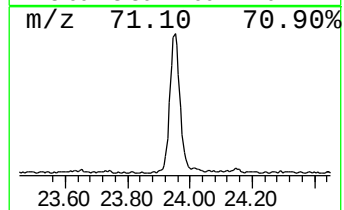
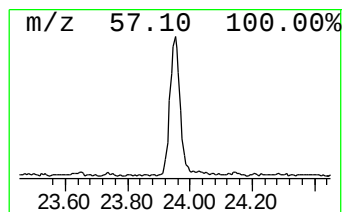
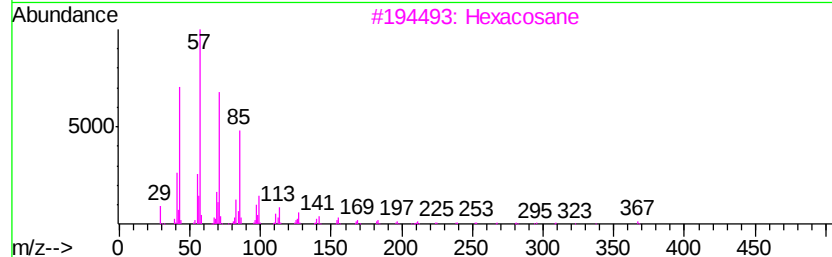
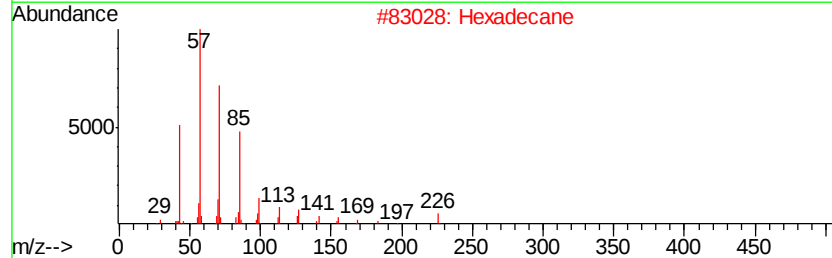
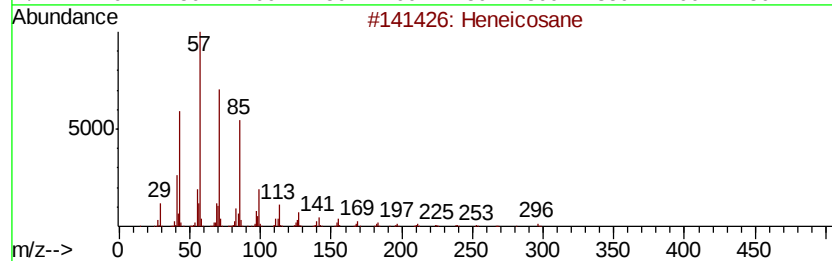
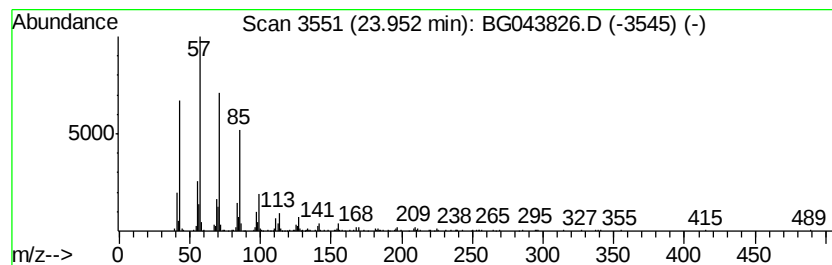
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.95	4.47 ng	450836	Perylene-d12	24.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	98
2	Hexadecane		226	C16H34	000544-76-3	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	Tetracosane		338	C24H50	000646-31-1	91
5	Heneicosane, 11-decyl-		437	C31H64	055320-06-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043826.D
Acq On : 17 Dec 2019 19:20
Operator : JU
Sample : K6294-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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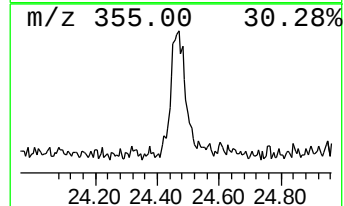
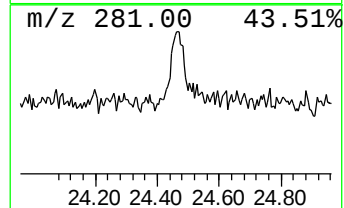
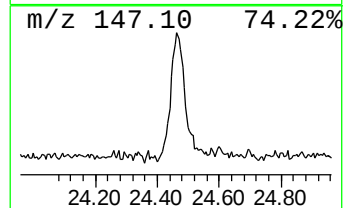
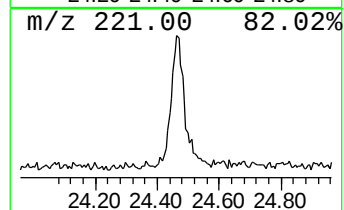
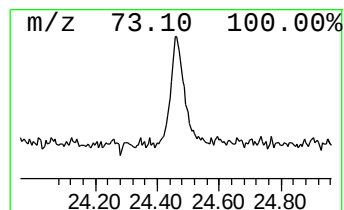
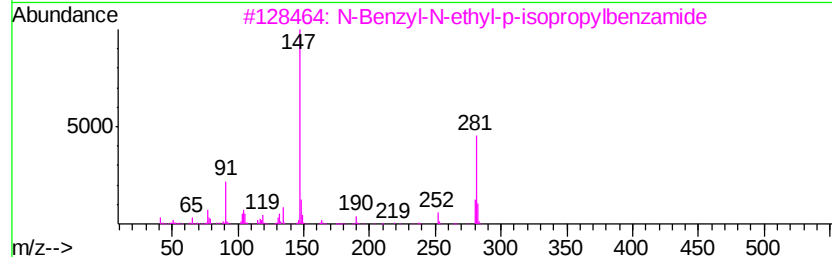
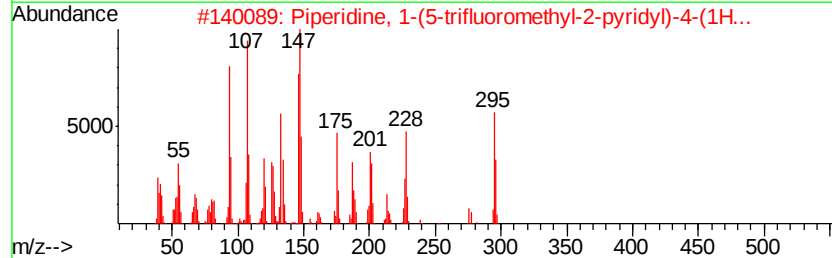
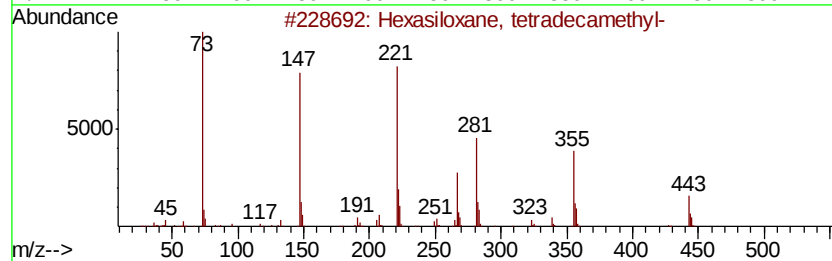
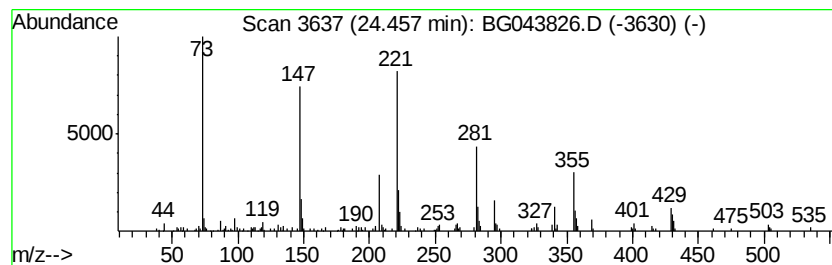
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexasiloxane, tetradecamethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.46	2.63 ng	264650	Perylene-d12	24.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	80
2		Piperidine, 1-(5-trifluoromethyl-2-pyridyl)-4-(1H...	295	C15H16F3N3	1000268-74-7	56
3		N-Benzyl-N-ethyl-p-isopropylbenzamide	281	C19H23NO	015089-22-2	27
4		(E)-2-Hydroxy-4'-cyano-stilbene	221	C15H11NO	1000147-85-5	27
5		Trisiloxane, 1,1,1,5,5,5-hexamethyl-	384	C12H36O4Si5	003555-47-3	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043826.D
Acq On : 17 Dec 2019 19:20
Operator : JU
Sample : K6294-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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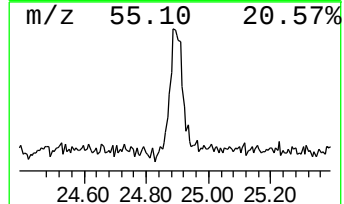
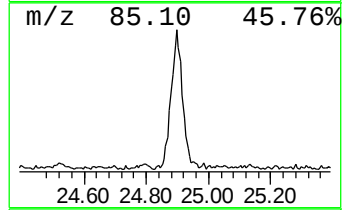
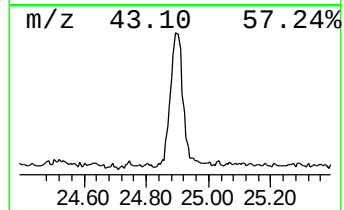
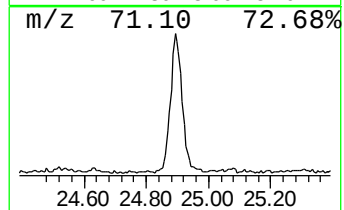
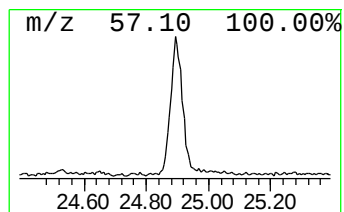
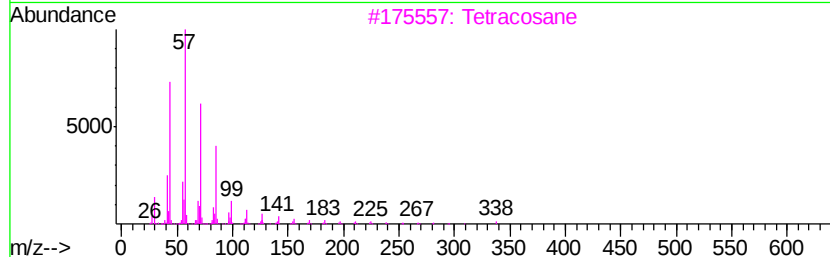
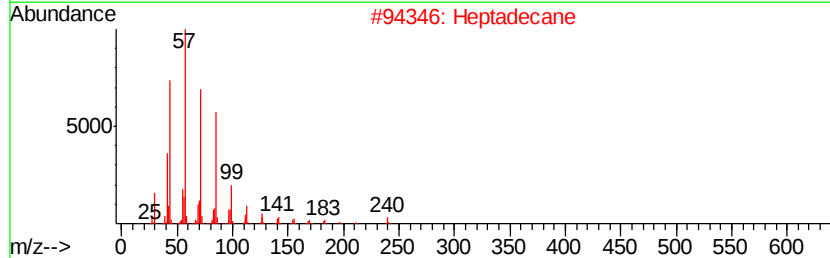
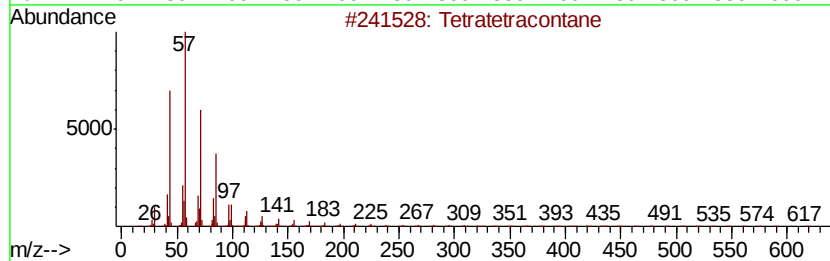
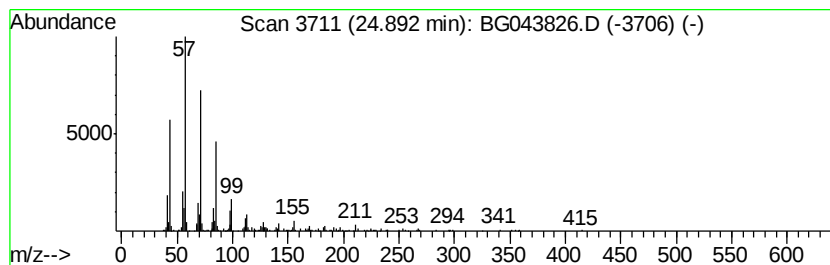
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.89	4.49 ng	452876	Perylene-d12	24.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Heptadecane	240	C17H36	000629-78-7	90
3			Tetracosane	338	C24H50	000646-31-1	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121719\
Data File : BG043826.D
Acq On : 17 Dec 2019 19:20
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Sample : K6294-01
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Instrument :
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ClientSampleId :
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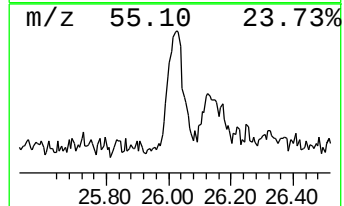
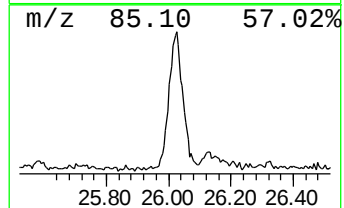
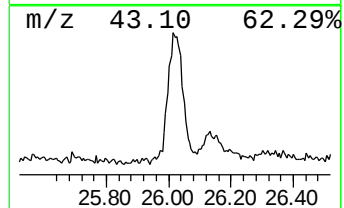
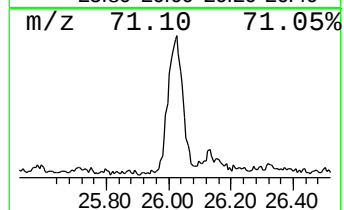
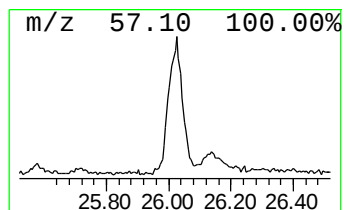
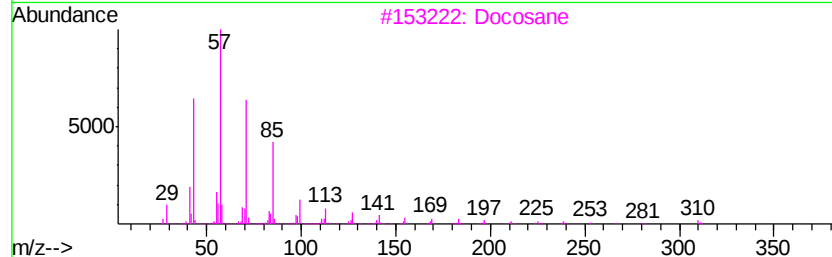
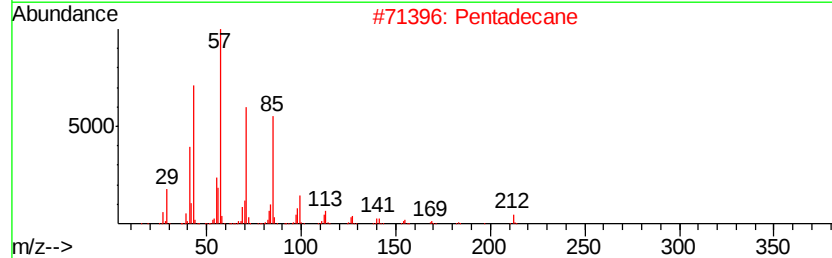
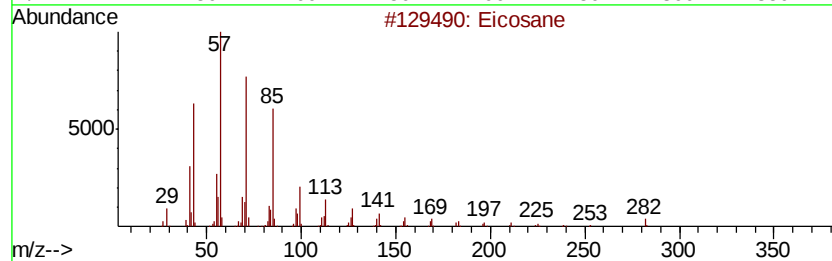
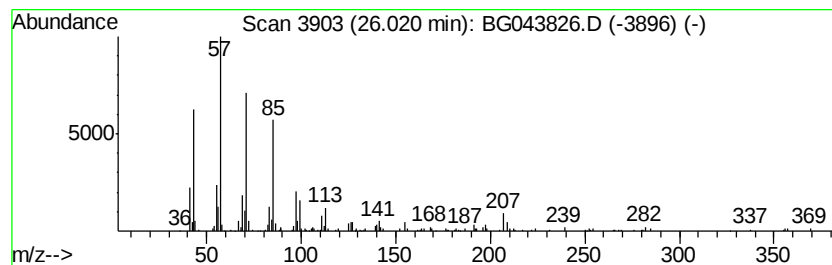
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.02	3.08 ng	310478	Perylene-d12	24.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	90
2		Pentadecane	212	C15H32	000629-62-9	74
3		Docosane	310	C22H46	000629-97-0	72
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	72
5		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121719\
Data File : BG043826.D
Acq On : 17 Dec 2019 19:20
Operator : JU
Sample : K6294-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG120919.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
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2-Pentanone, 4-hy...	5.12	20.1	ng	626109	1	8.00	624320	20.0
unknown7.54	7.54	105.1	ng	3279590	1	8.00	624320	20.0
2-Chloropropioni...	21.30	7.3	ng	818957	5	21.63	2247510	20.0
Octadecane	21.85	2.0	ng	226180	5	21.63	2247510	20.0
Eicosane, 10-methyl-	22.46	4.1	ng	464236	5	21.63	2247510	20.0
2-methyloctacosane	23.15	3.9	ng	438065	5	21.63	2247510	20.0
Heneicosane	23.95	4.5	ng	450836	6	24.79	2015210	20.0
Hexasiloxane, tet...	24.46	2.6	ng	264650	6	24.79	2015210	20.0
Tetratetracontane	24.89	4.5	ng	452876	6	24.79	2015210	20.0
Pentadecane	26.02	3.1	ng	310478	6	24.79	2015210	20.0