

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
 Data File : BG043689.D
 Acq On : 19 Nov 2019 1:28
 Operator : JU
 Sample : K5833-12
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 8-(2-4)

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	3.158	6	12	19	rVB	72508	123058	5.29%	0.959%
2	5.097	337	342	358	rVB	94472	151256	6.50%	1.178%
3	5.585	418	425	444	rBV	432406	768639	33.02%	5.989%
4	7.189	691	698	709	rBV	468302	895500	38.47%	6.977%
5	7.535	749	757	770	rBV	489485	863865	37.11%	6.731%
6	7.993	828	835	843	rBV	94416	170556	7.33%	1.329%
7	8.317	882	890	900	rBV	367452	669049	28.74%	5.213%
8	9.157	1025	1033	1051	rBV	244879	518940	22.30%	4.043%
9	10.796	1306	1312	1322	rBV	95544	202395	8.70%	1.577%
10	13.246	1722	1729	1748	rBV	742109	1251618	53.77%	9.752%
11	14.075	1865	1870	1884	rBV	76990	144427	6.21%	1.125%
12	14.627	1957	1964	1979	rVB2	196861	342117	14.70%	2.666%
13	16.113	2210	2217	2234	rBV	694978	1195521	51.36%	9.315%
14	16.319	2244	2252	2268	rBV	177041	319954	13.75%	2.493%
15	17.371	2422	2431	2441	rBV	273557	446747	19.19%	3.481%
16	18.264	2578	2583	2591	rBV3	34602	56254	2.42%	0.438%
17	19.979	2869	2875	2886	rBV	1723387	2327555	100.00%	18.135%
18	21.278	3091	3096	3111	rBV5	32762	102459	4.40%	0.798%
19	21.636	3150	3157	3169	rBV2	293050	575428	24.72%	4.483%
20	21.813	3182	3187	3195	rBV2	51762	73977	3.18%	0.576%
21	22.412	3283	3289	3295	rBV	82630	127575	5.48%	0.994%
22	23.093	3398	3405	3412	rBV	105134	185118	7.95%	1.442%
23	23.281	3433	3437	3443	rVB6	14301	26008	1.12%	0.203%
24	23.881	3532	3539	3547	rVB2	100729	203359	8.74%	1.584%
25	24.815	3686	3698	3716	rBV2	287797	834041	35.83%	6.498%
26	25.914	3874	3885	3895	rBV3	59450	172867	7.43%	1.347%
27	27.236	4104	4110	4120	rVB5	27368	86626	3.72%	0.675%

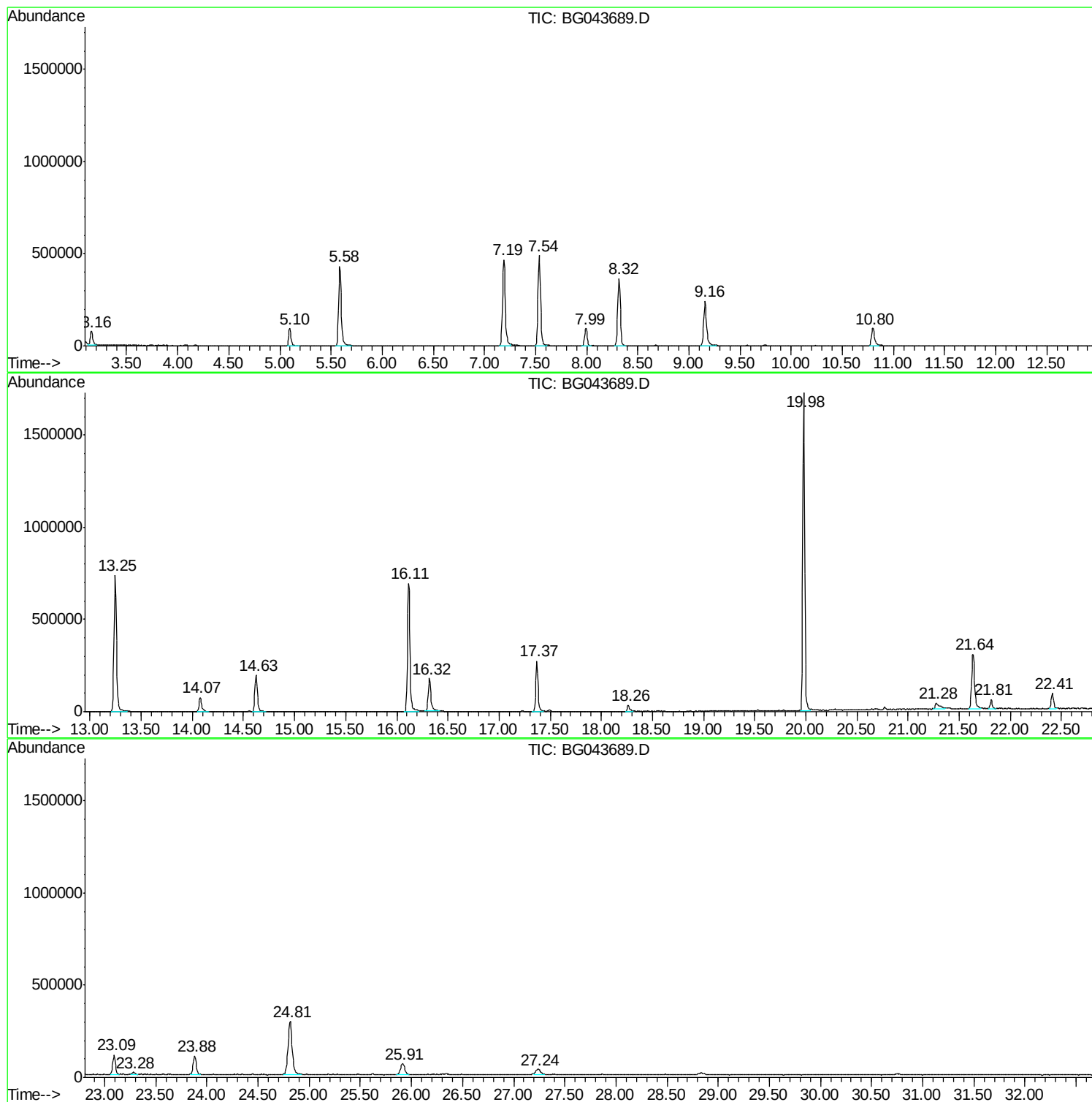
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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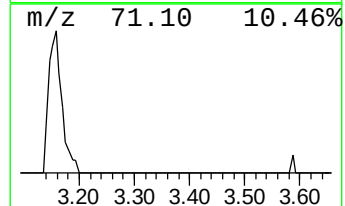
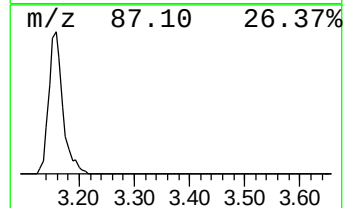
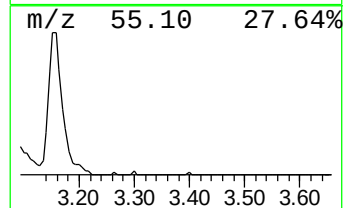
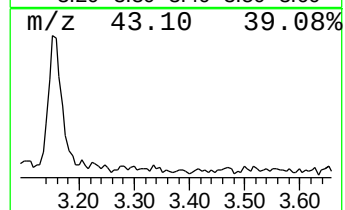
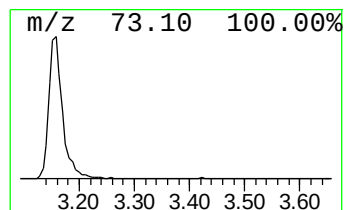
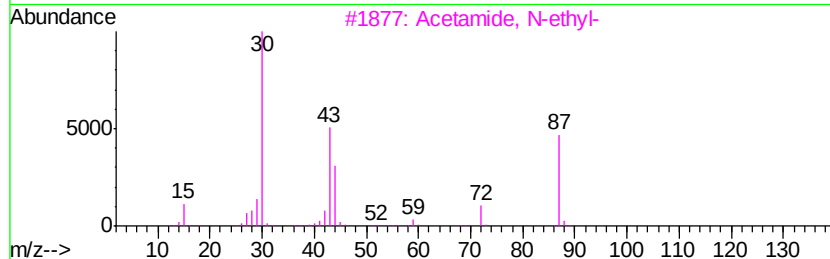
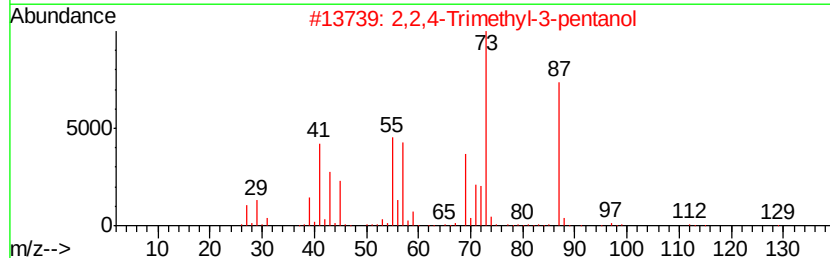
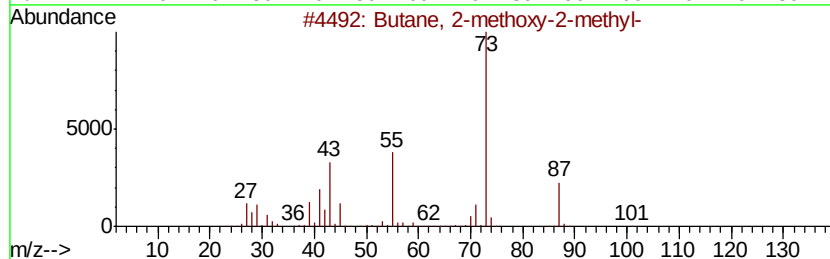
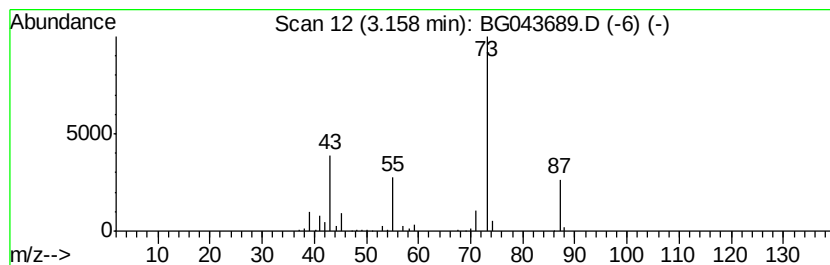
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	14.43 ng	123058	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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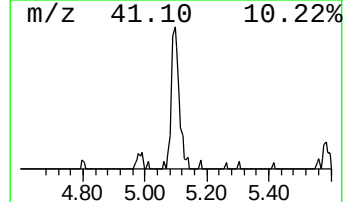
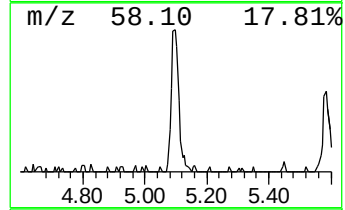
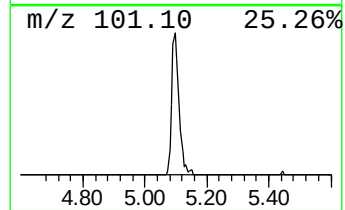
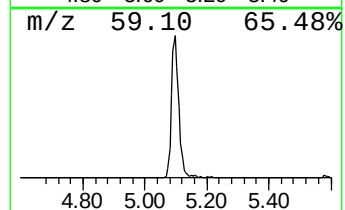
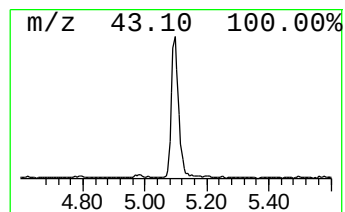
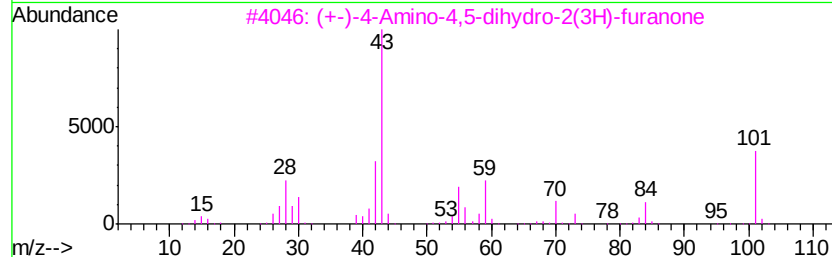
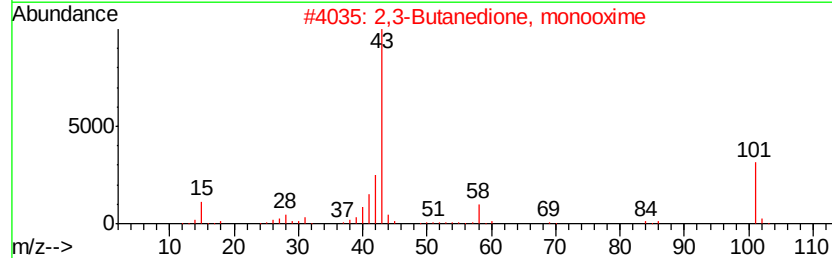
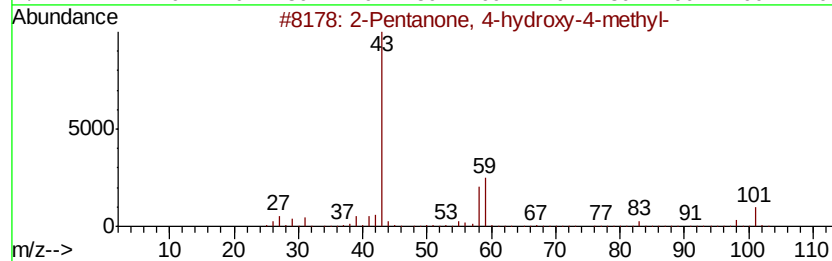
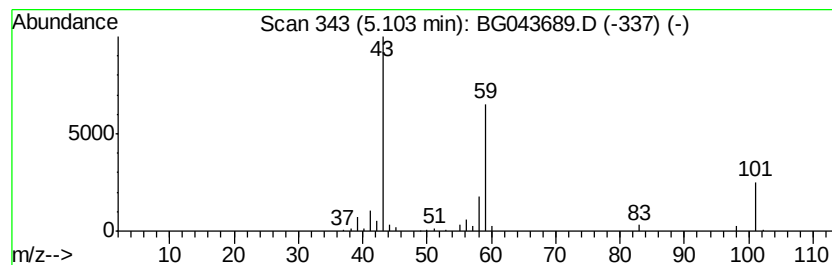
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	17.74 ng	151256	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	23
4		Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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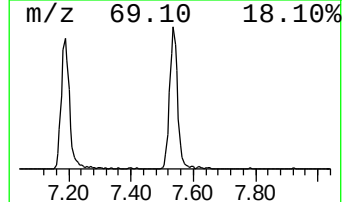
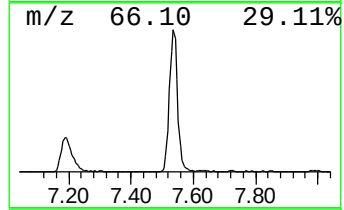
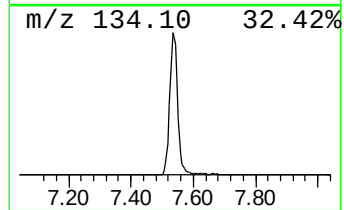
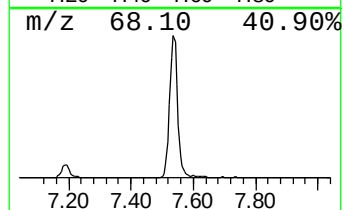
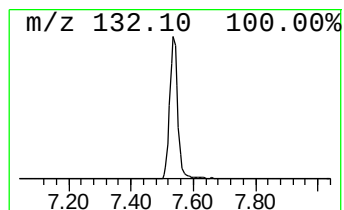
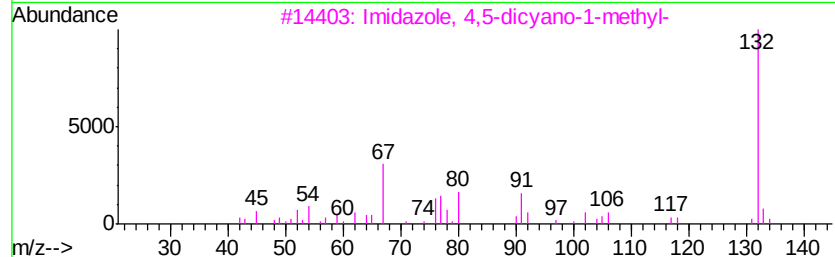
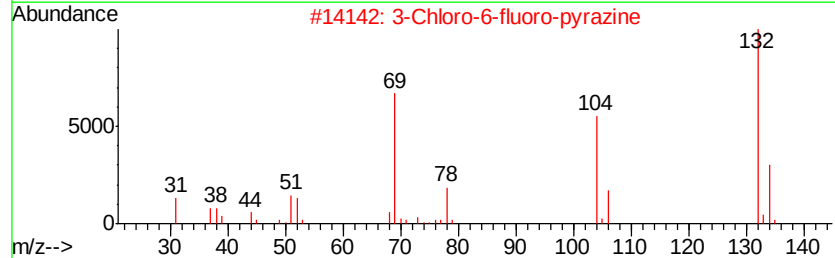
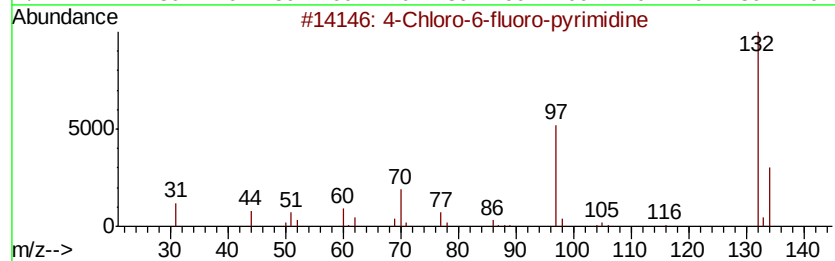
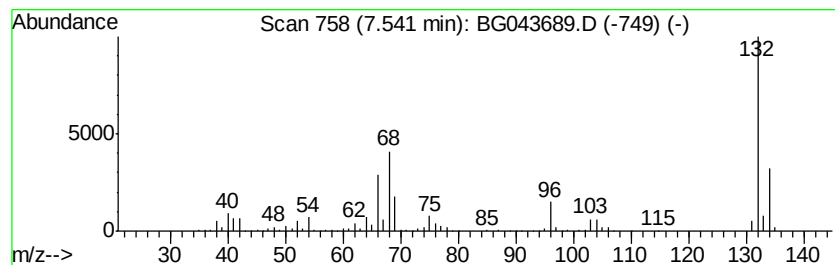
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Peak Number 3 unknown7.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	101.30 ng	863865	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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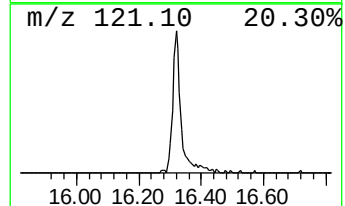
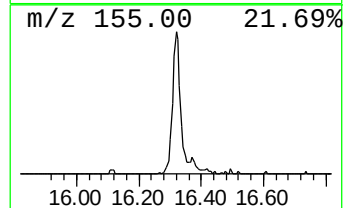
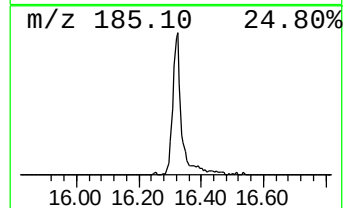
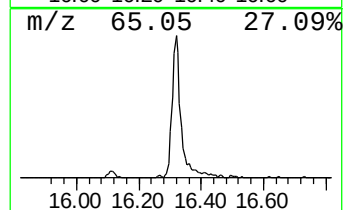
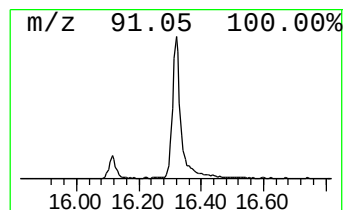
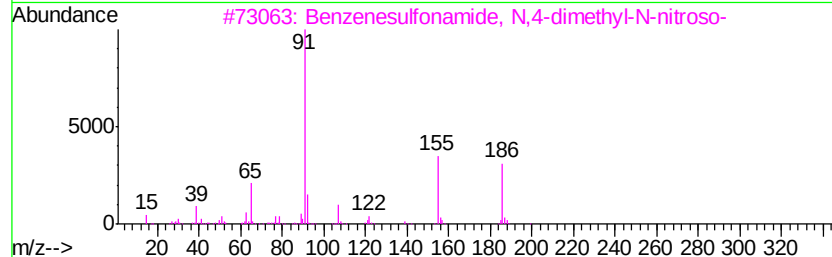
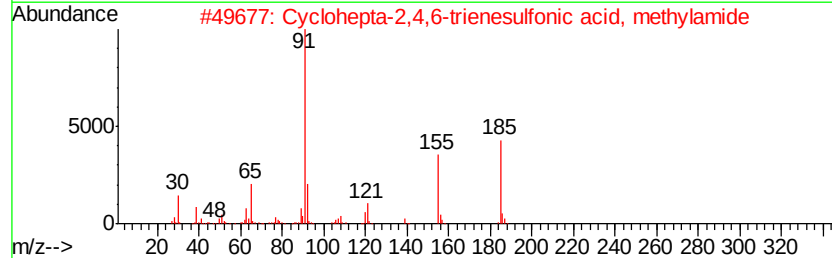
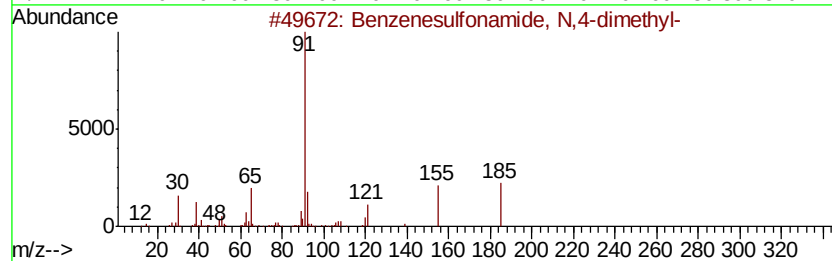
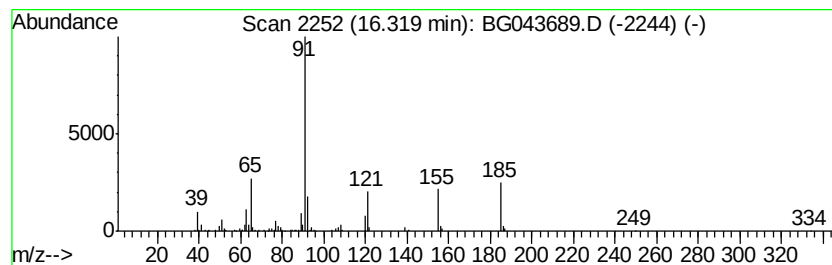
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Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	14.32 ng	319954	Phenanthrene-d10	17.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	90
2		Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	64
3		Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	53
4		N-Sulfinyl-p-toluenesulfonamide	217	C7H7NO3S2	004104-47-6	50
5		Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	49



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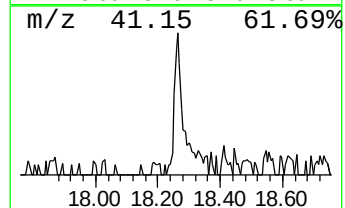
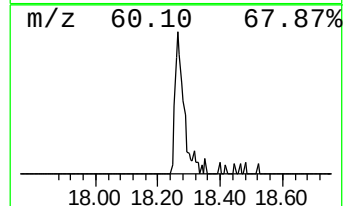
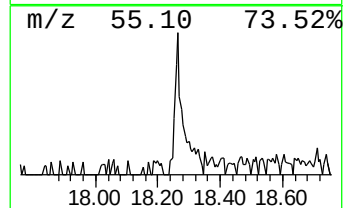
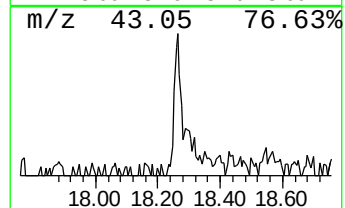
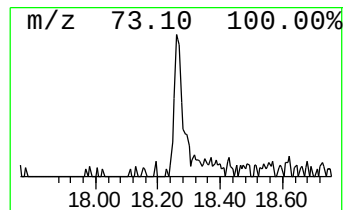
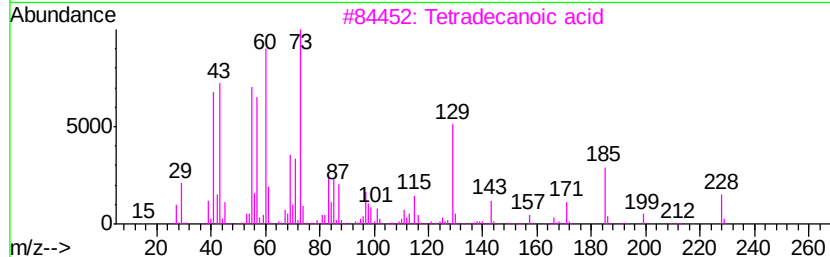
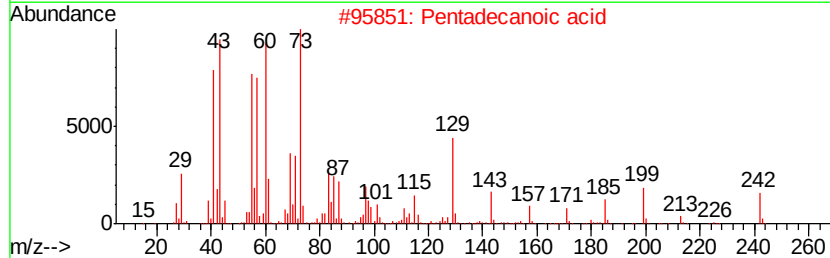
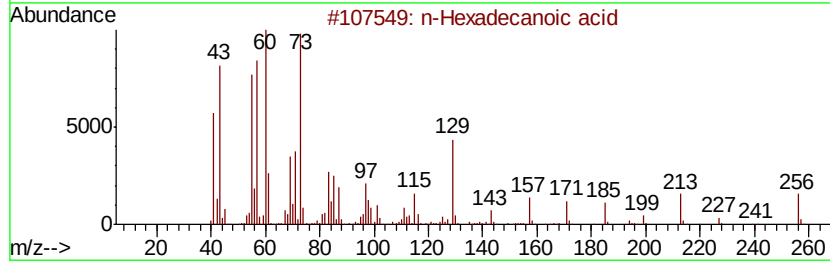
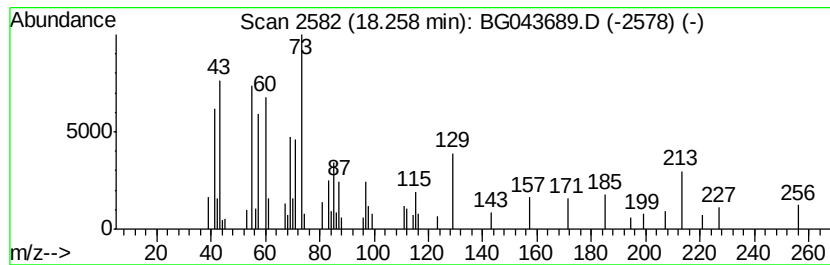
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.26	2.52 ng	56254	Phenanthrene-d10	17.37		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4		Tridecanoic acid	214	C13H26O2	000638-53-9	59
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



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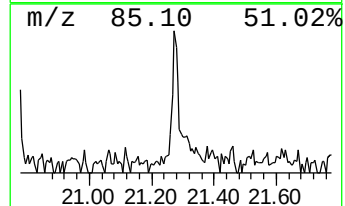
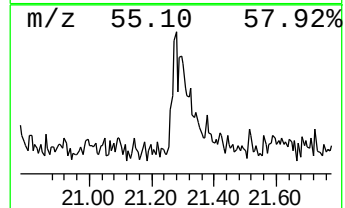
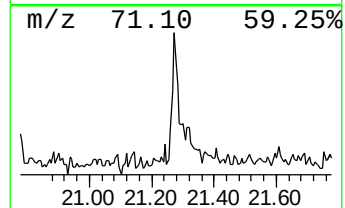
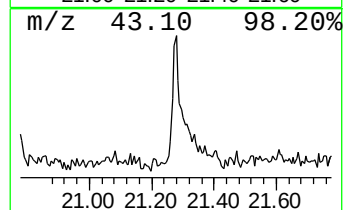
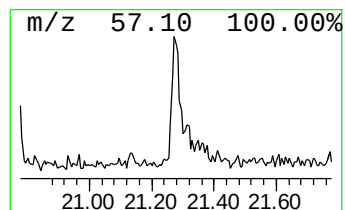
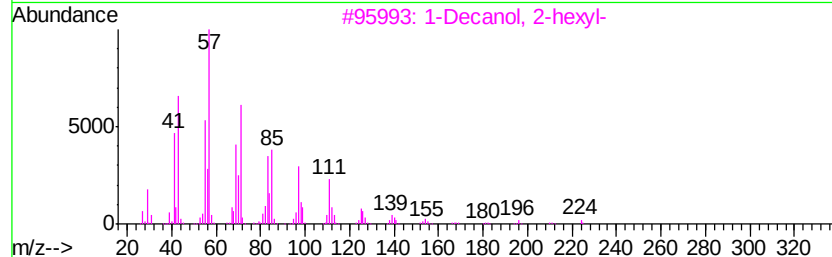
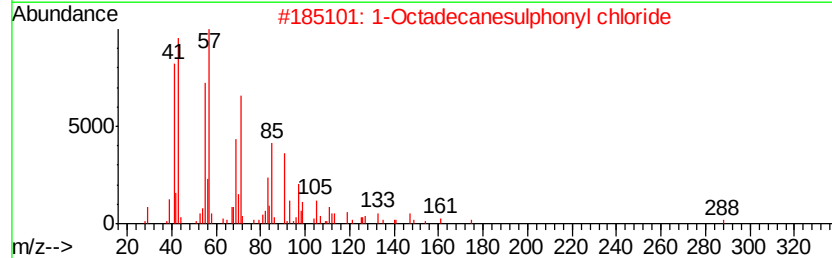
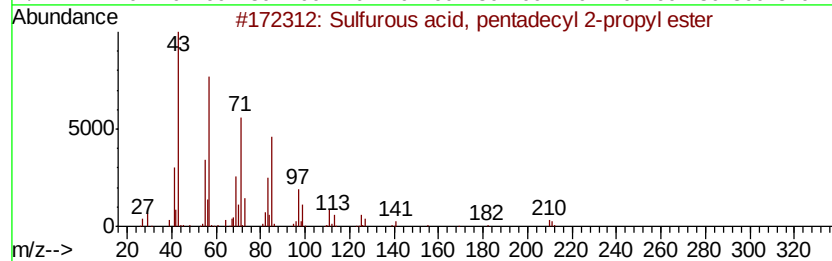
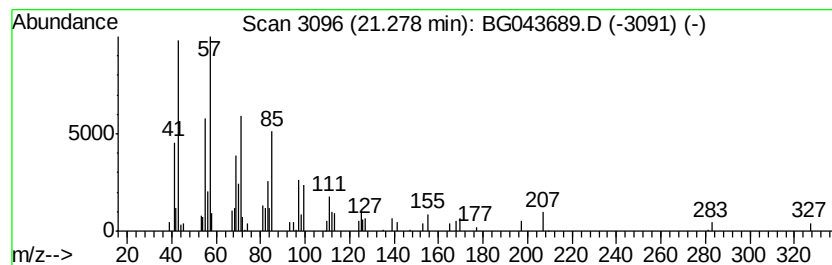
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, pentadecyl ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.28	3.56 ng	102459	Chrysene-d12	21.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	72
2			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	64
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	58
4			Pentadecane	212	C15H32	000629-62-9	52
5			2-methyltetracosane	352	C25H52	1000376-72-6	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043689.D
Acq On : 19 Nov 2019 1:28
Operator : JU
Sample : K5833-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

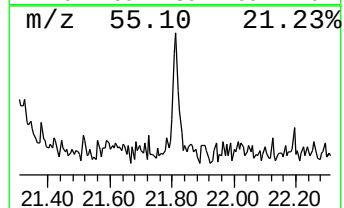
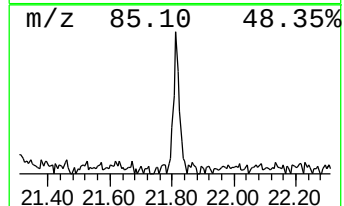
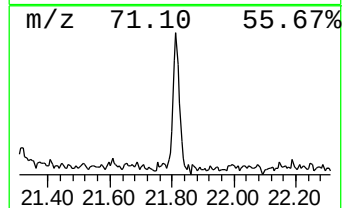
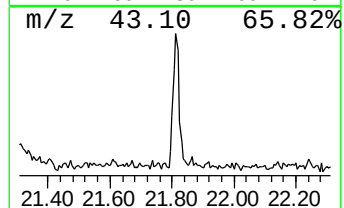
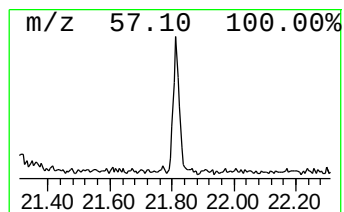
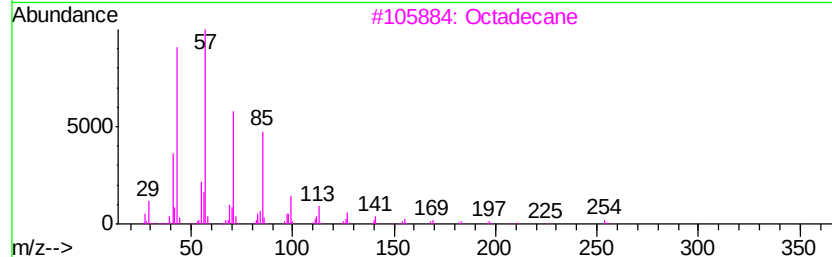
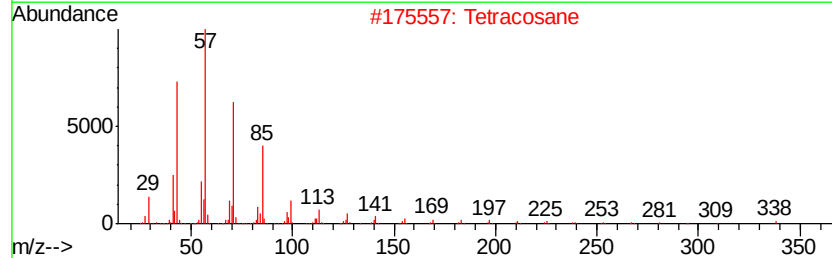
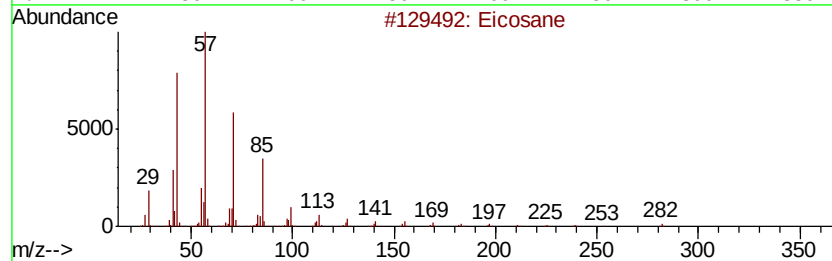
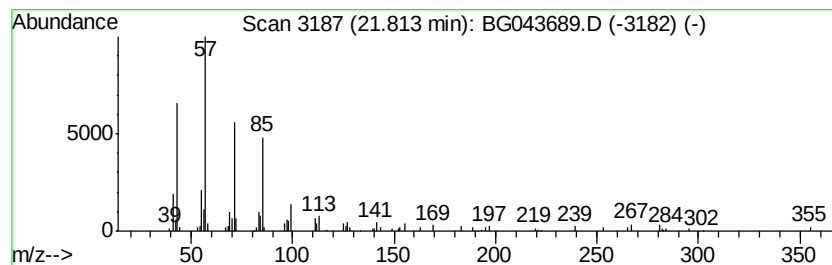
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.81	2.57 ng	73977	Chrysene-d12		21.63	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	96
2	Tetracosane		338	C24H50	000646-31-1	83
3	Octadecane		254	C18H38	000593-45-3	83
4	Octacosane		394	C28H58	000630-02-4	80
5	Tetradecane		198	C14H30	000629-59-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043689.D
Acq On : 19 Nov 2019 1:28
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ClientSampleId :
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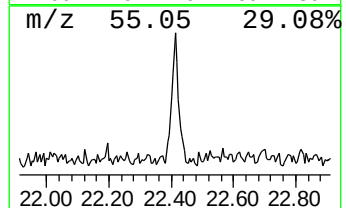
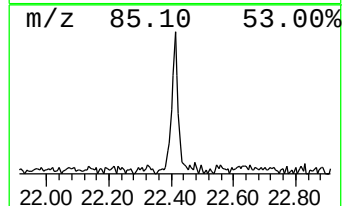
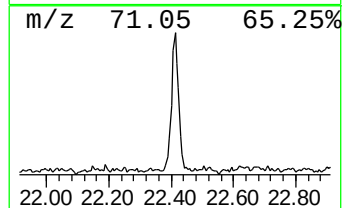
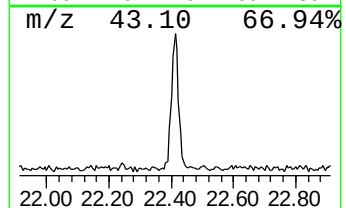
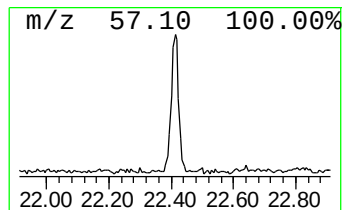
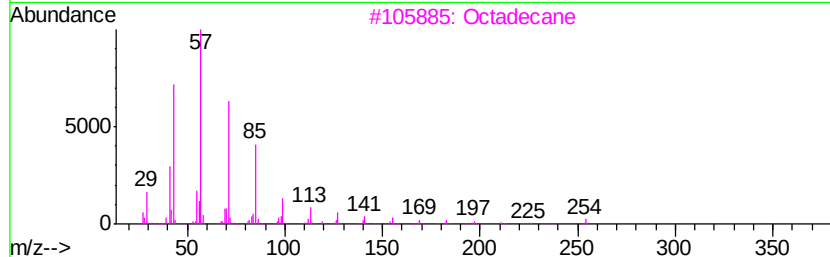
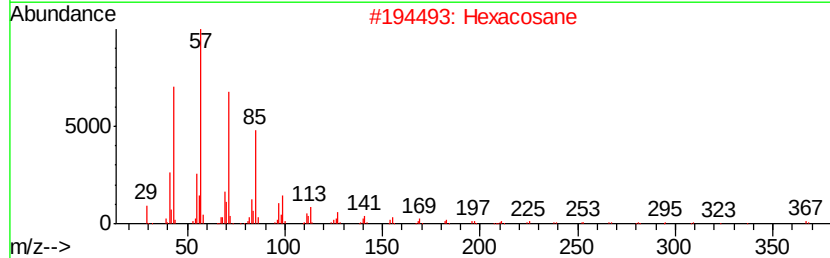
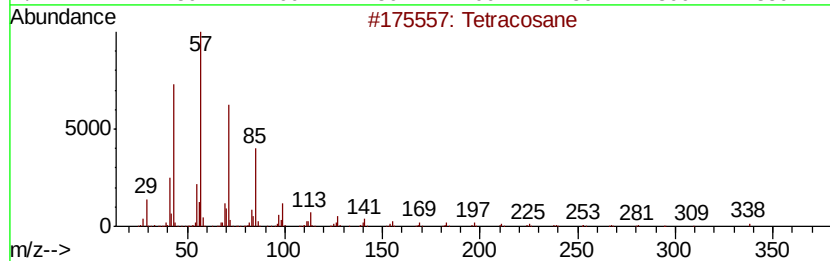
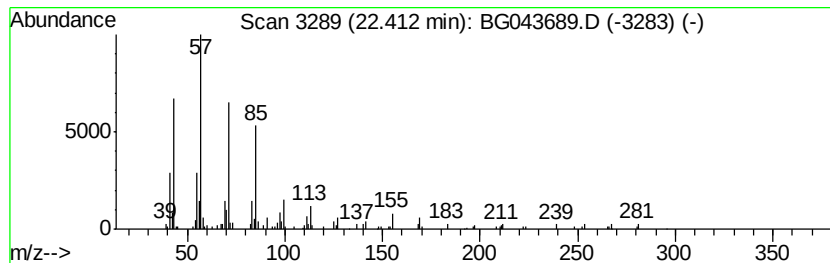
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	4.43 ng	127575	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		Octadecane	254	C18H38	000593-45-3	87
4		Pentacosane	352	C25H52	000629-99-2	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043689.D
Acq On : 19 Nov 2019 1:28
Operator : JU
Sample : K5833-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

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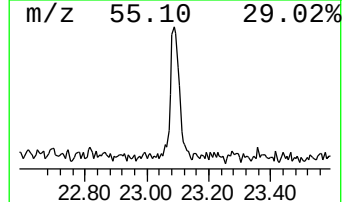
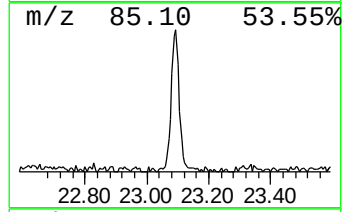
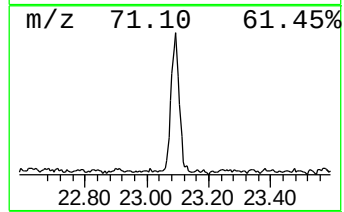
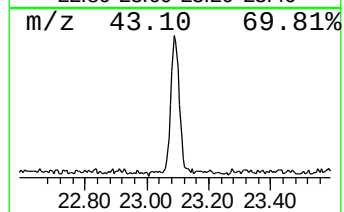
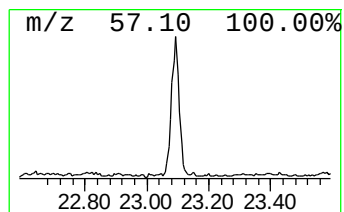
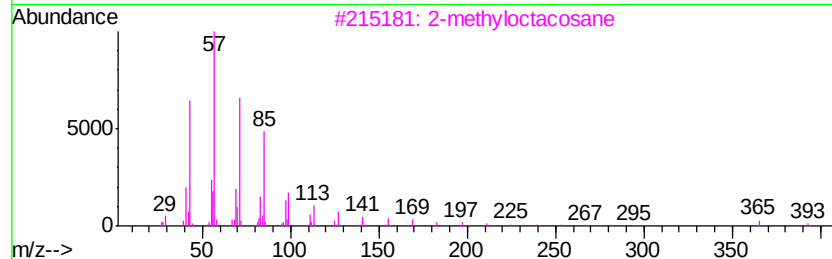
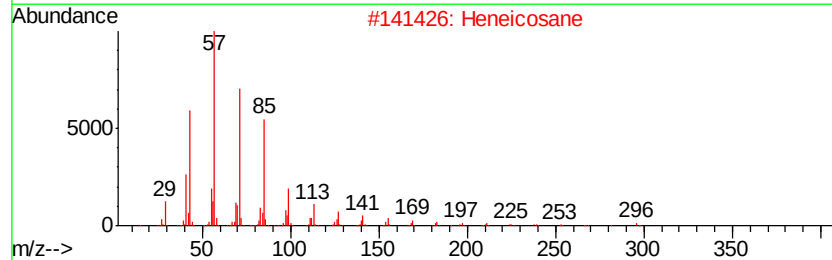
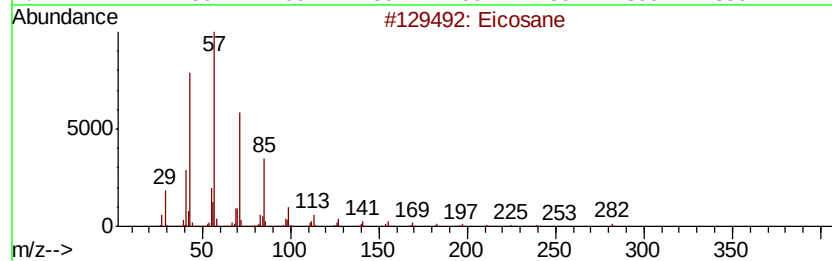
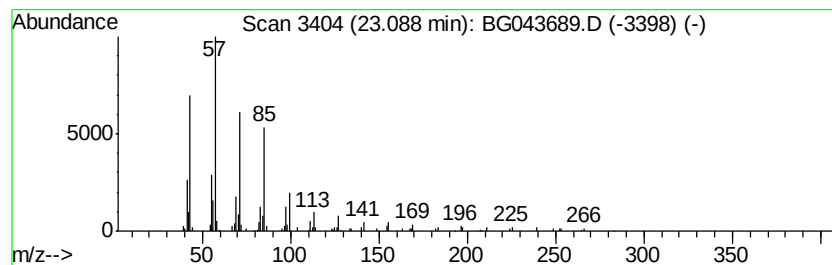
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	6.43 ng	185118	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Heneicosane	296	C21H44	000629-94-7	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Hentriacontane	437	C31H64	000630-04-6	90
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043689.D
Acq On : 19 Nov 2019 1:28
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Sample : K5833-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

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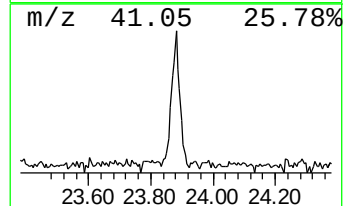
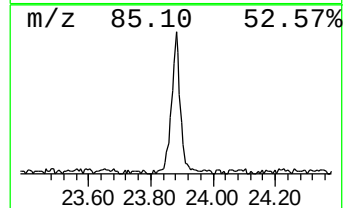
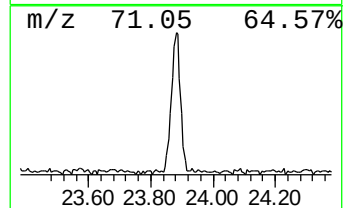
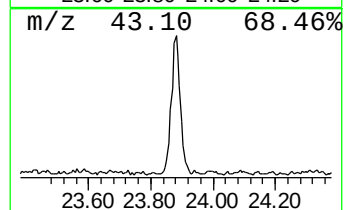
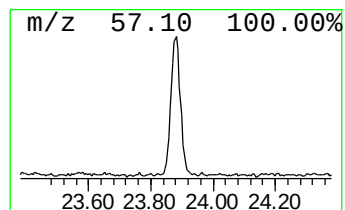
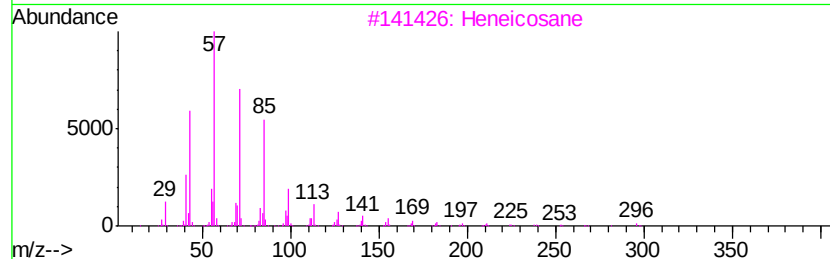
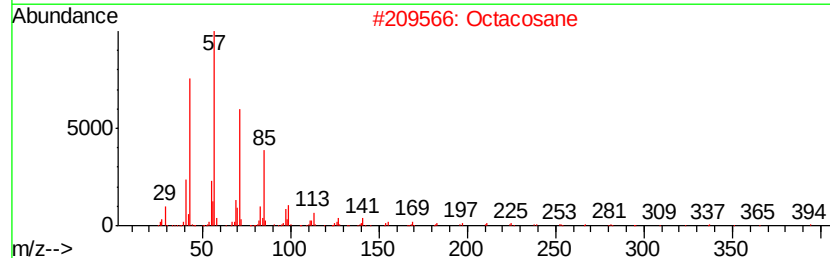
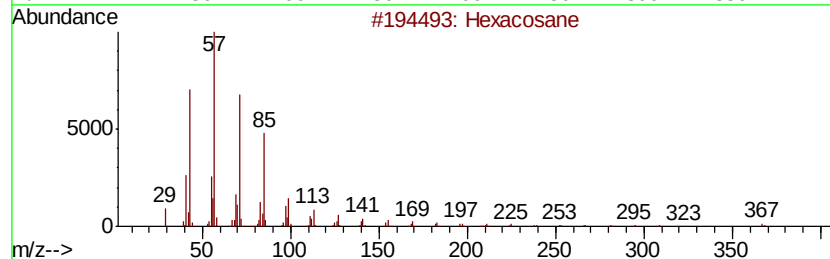
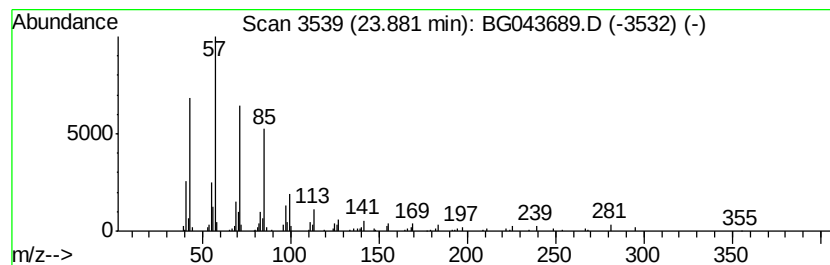
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.88	4.88 ng	203359	Perylene-d12	24.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Eicosane, 2-methyl-	296	C21H44	001560-84-5	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043689.D
Acq On : 19 Nov 2019 1:28
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Misc :
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Instrument :
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ClientSampleId :
8-(2-4)

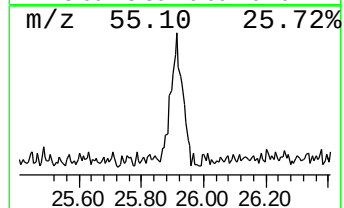
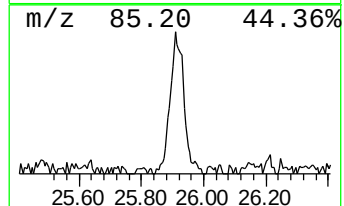
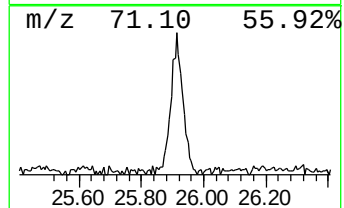
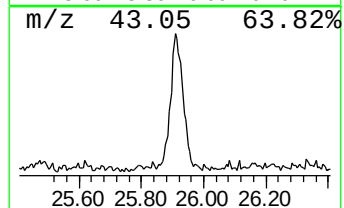
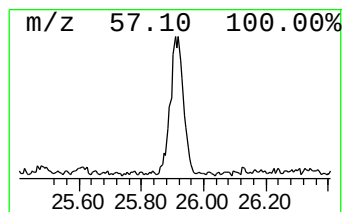
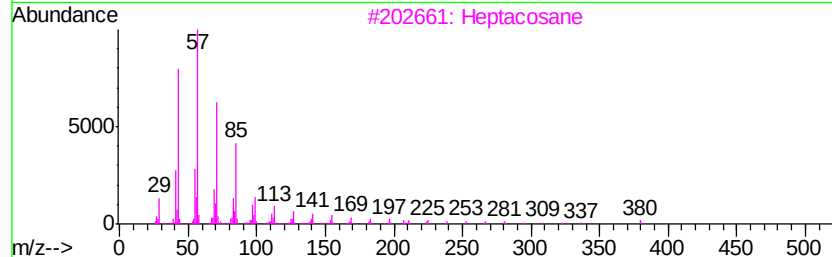
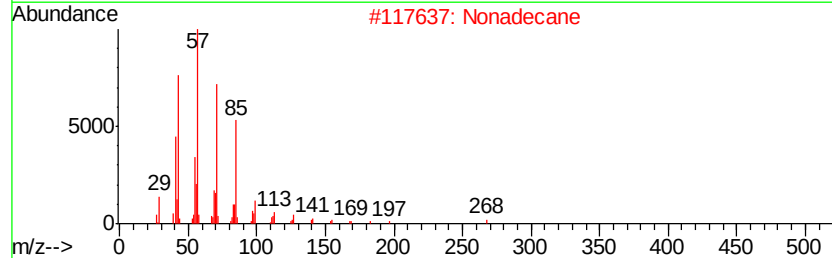
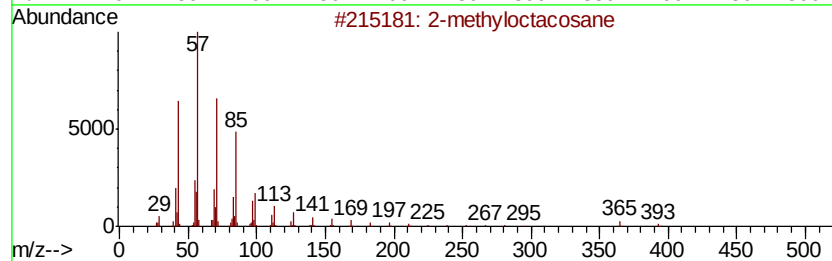
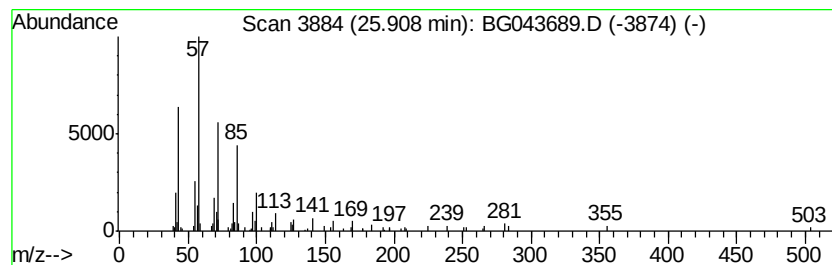
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	4.15 ng	172867	Perylene-d12	24.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Nonadecane	268	C19H40	000629-92-5	90
3			Heptacosane	380	C27H56	000593-49-7	90
4			Docosane, 11-butyl-	366	C26H54	013475-76-8	87
5			Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111819\
Data File : BG043689.D
Acq On : 19 Nov 2019 1:28
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Sample : K5833-12
Misc :
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Instrument :
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ClientSampleId :
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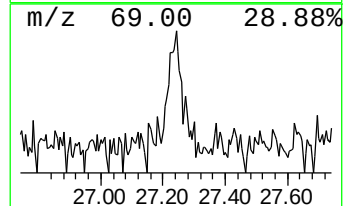
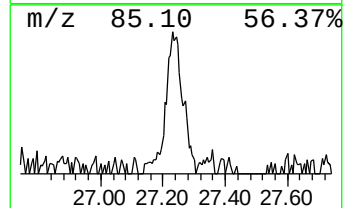
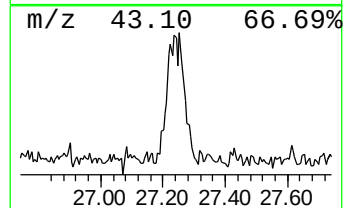
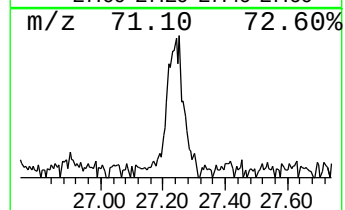
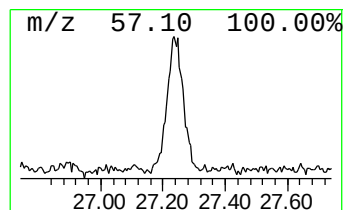
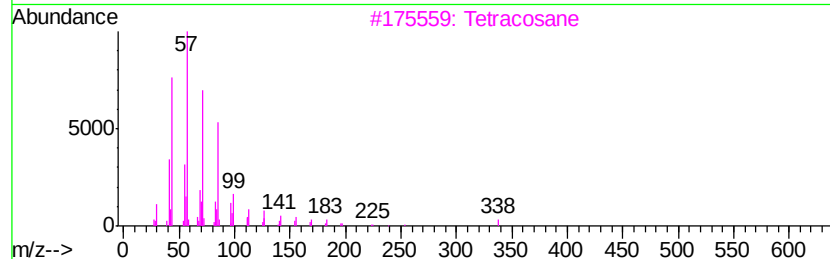
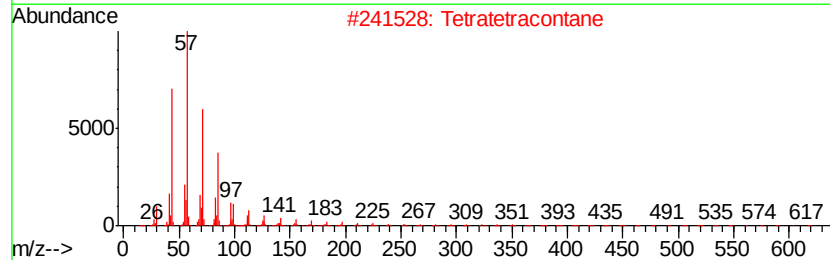
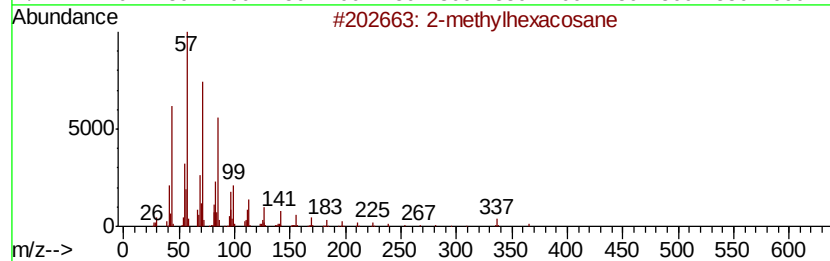
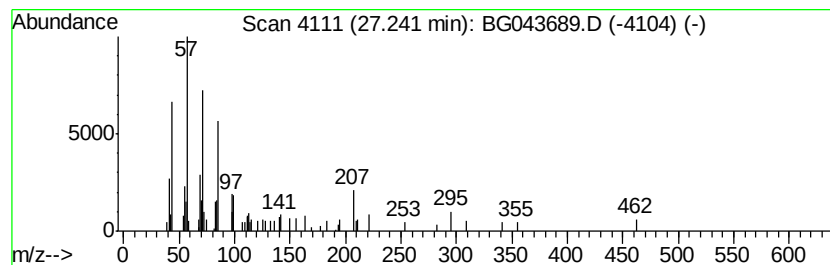
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-methylhexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.24	2.08 ng	86626	Perylene-d12	24.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methylhexacosane	380	C27H56	1000376-72-7	72
2		Tetratetracontane	619	C44H90	007098-22-8	72
3		Tetracosane	338	C24H50	000646-31-1	64
4		Hexacosane	366	C26H54	000630-01-3	64
5		Hentriacontane	437	C31H64	000630-04-6	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111819\
Data File : BG043689.D
Acq On : 19 Nov 2019 1:28
Operator : JU
Sample : K5833-12
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
8-(2-4)

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
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2-Pentanone, 4-hy...	5.10	17.7	ng	151256	1	7.99	170556	20.0
unknown7.54	7.54	101.3	ng	863865	1	7.99	170556	20.0
Benzenesulfonamid...	16.32	14.3	ng	319954	4	17.37	446747	20.0
n-Hexadecanoic acid	18.26	2.5	ng	56254	4	17.37	446747	20.0
Sulfurous acid, p...	21.28	3.6	ng	102459	5	21.63	575428	20.0
Eicosane	21.81	2.6	ng	73977	5	21.63	575428	20.0
Tetracosane	22.41	4.4	ng	127575	5	21.63	575428	20.0
Heneicosane	23.09	6.4	ng	185118	5	21.63	575428	20.0
Hexacosane	23.88	4.9	ng	203359	6	24.81	834041	20.0
2-methyloctacosane	25.91	4.2	ng	172867	6	24.81	834041	20.0
2-methylhexacosane	27.24	2.1	ng	86626	6	24.81	834041	20.0