

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
 Data File : BG040432.D
 Acq On : 11 Apr 2019 3:45
 Operator : JU/SJ
 Sample : K2311-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 0237-COMP-CS-2-ELTRT

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-BG032719.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	3.178	13	15	24	rVB2	33099	53160	2.32%	0.411%
2	5.599	420	427	437	rBV	207686	347027	15.13%	2.685%
3	7.197	692	699	711	rBV	170551	322927	14.08%	2.499%
4	7.573	756	763	771	rBV	356742	609100	26.56%	4.713%
5	8.043	834	843	855	rBV	128016	225839	9.85%	1.747%
6	8.366	891	898	906	rBV	329427	578280	25.21%	4.475%
7	9.218	1035	1043	1053	rBV	271153	520501	22.69%	4.027%
8	10.858	1315	1322	1336	rBV	148854	289417	12.62%	2.239%
9	12.426	1583	1589	1594	rBV2	18647	27612	1.20%	0.214%
10	13.296	1727	1737	1748	rBV	674325	1119832	48.83%	8.665%
11	14.124	1872	1878	1884	rBV	65261	102341	4.46%	0.792%
12	14.677	1964	1972	1980	rBV2	255176	425044	18.53%	3.289%
13	16.163	2219	2225	2241	rBV	528368	902374	39.34%	6.982%
14	17.421	2431	2439	2446	rBV2	395240	620915	27.07%	4.804%
15	17.697	2481	2486	2488	rBV2	33040	50023	2.18%	0.387%
16	17.732	2488	2492	2500	rVB	45890	74582	3.25%	0.577%
17	18.278	2580	2585	2592	rBV2	73827	130395	5.69%	1.009%
18	19.547	2797	2801	2807	rBV7	20464	37833	1.65%	0.293%
19	19.788	2831	2842	2843	rBV7	44579	83372	3.64%	0.645%
20	20.023	2876	2882	2889	rVB	1669327	2293555	100.00%	17.747%
21	20.511	2960	2965	2973	rVB	16675	29336	1.28%	0.227%
22	20.781	3008	3011	3015	rBV5	20705	30907	1.35%	0.239%
23	20.852	3021	3023	3028	rVB6	17669	23615	1.03%	0.183%
24	21.298	3093	3099	3113	rBV3	130742	360135	15.70%	2.787%
25	21.545	3137	3141	3145	rVB4	19813	27940	1.22%	0.216%
26	21.692	3159	3166	3173	rBV	480669	821332	35.81%	6.355%
27	21.833	3186	3190	3196	rVB	85627	119476	5.21%	0.924%
28	22.444	3289	3294	3300	rVB	134651	206981	9.02%	1.602%
29	23.137	3406	3412	3423	rVB	204767	419703	18.30%	3.248%
30	23.942	3542	3549	3559	rVB2	177994	388848	16.95%	3.009%
31	24.900	3701	3712	3717	rBV2	147165	422557	18.42%	3.270%
32	24.965	3717	3723	3736	rVB3	250463	768926	33.53%	5.950%
33	26.034	3895	3905	3915	rBV4	110389	313048	13.65%	2.422%
34	27.391	4128	4136	4148	rVB4	51784	176850	7.71%	1.368%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 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-BG032719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

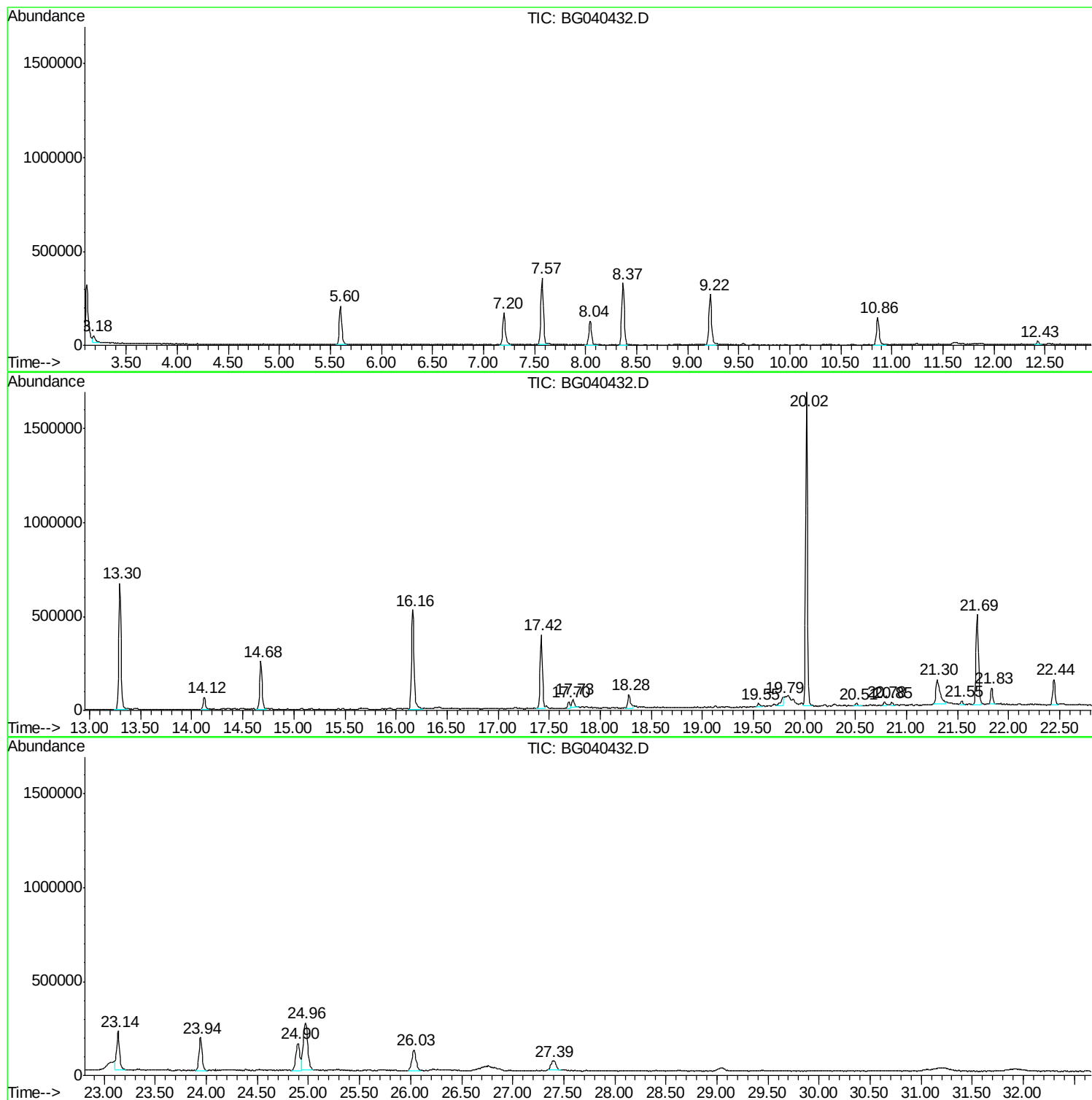
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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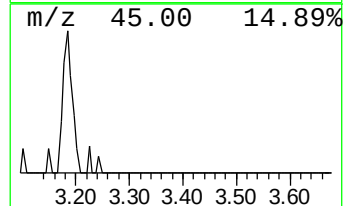
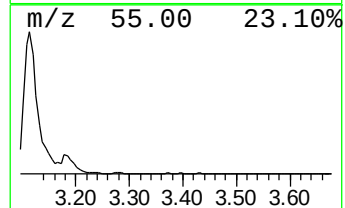
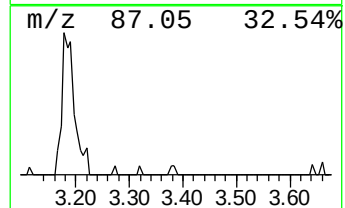
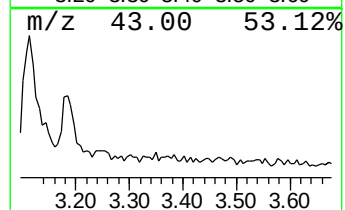
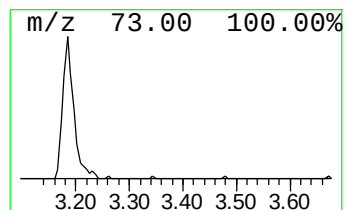
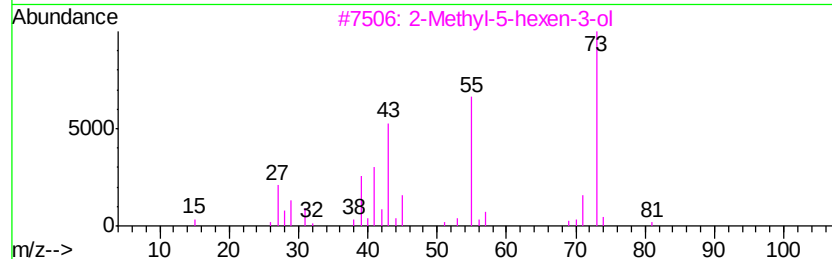
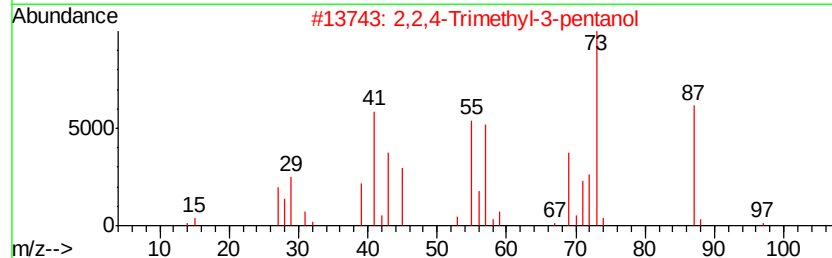
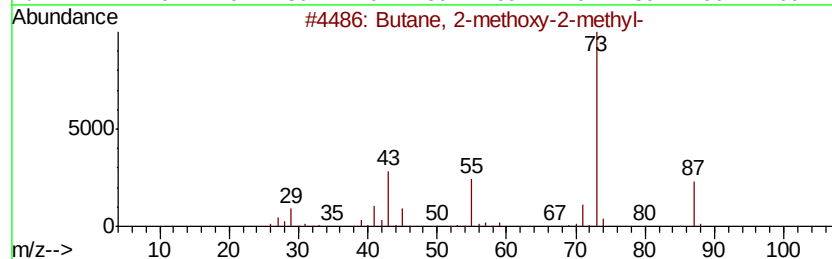
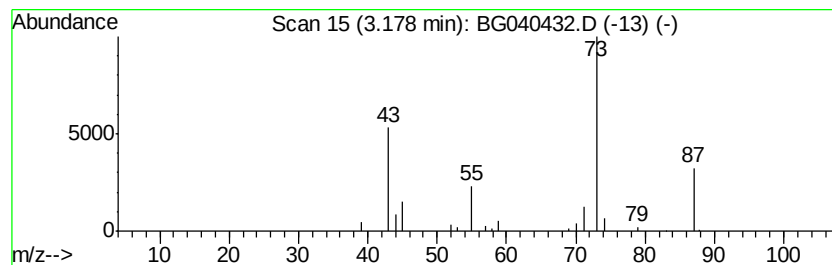
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	4.71 ng	53160	1,4-Dichlorobenzene-d4	8.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4			1,4-Butanediamine	88	C4H12N2	000110-60-1	10
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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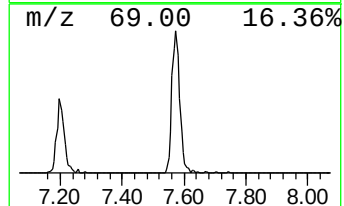
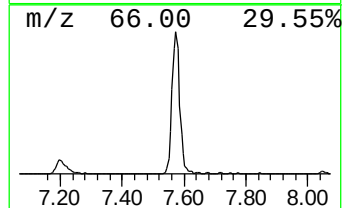
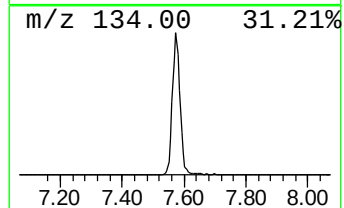
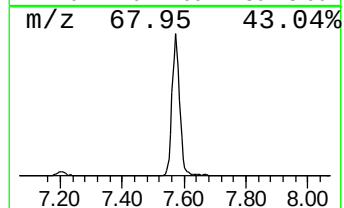
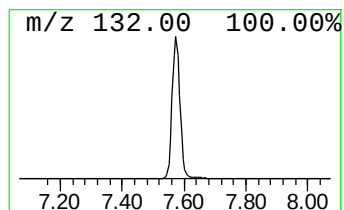
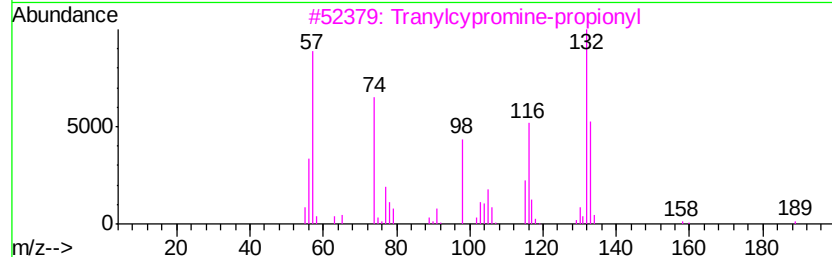
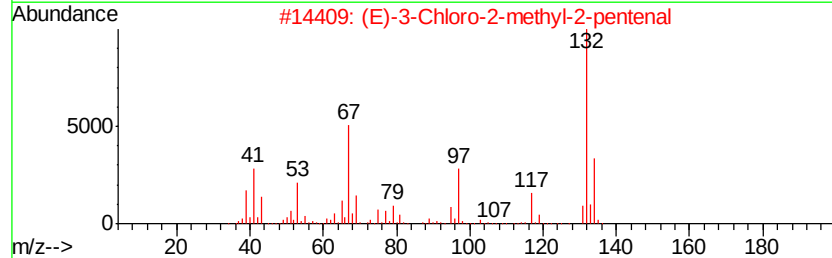
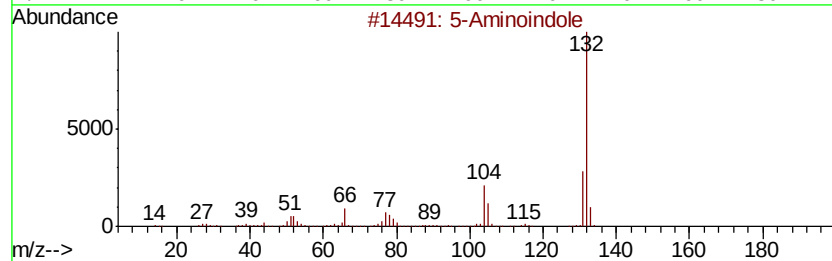
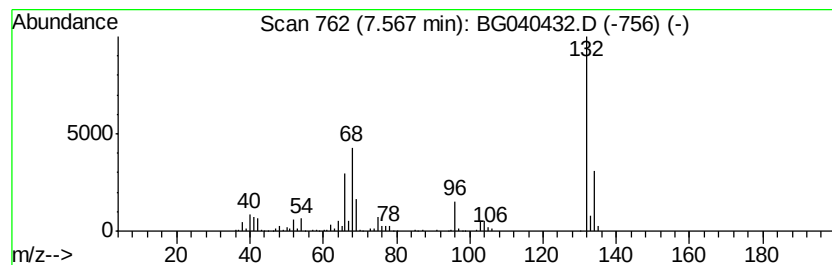
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG032719.M
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	53.94 ng	609100	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	22
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	10



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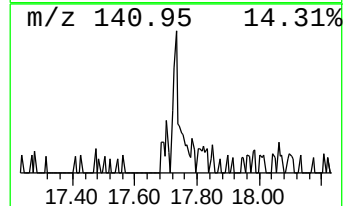
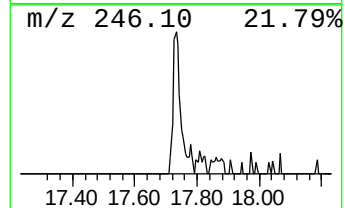
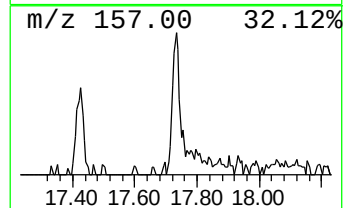
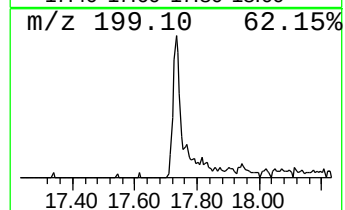
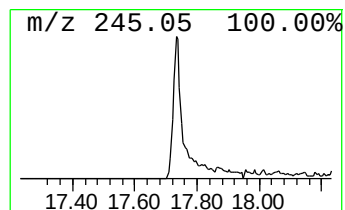
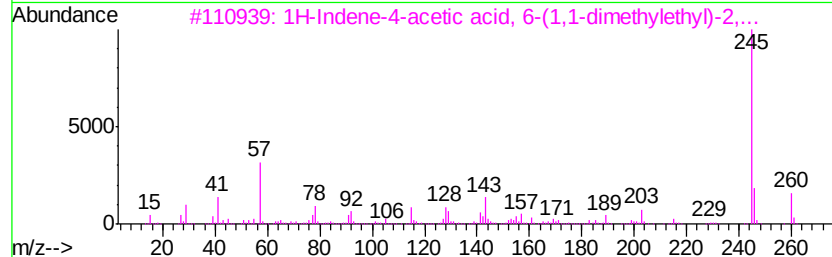
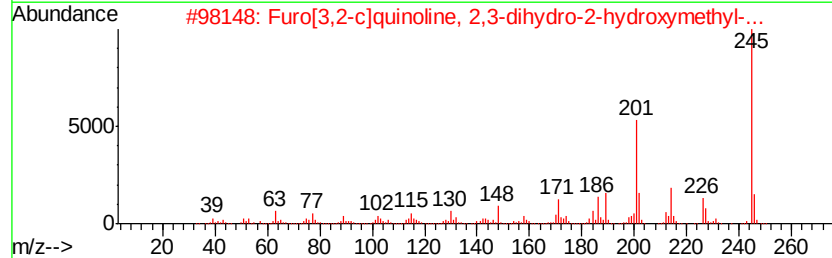
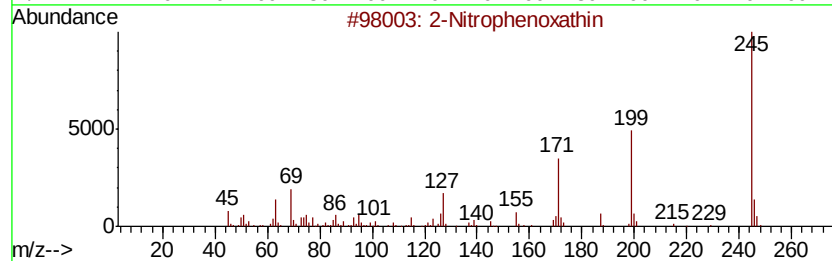
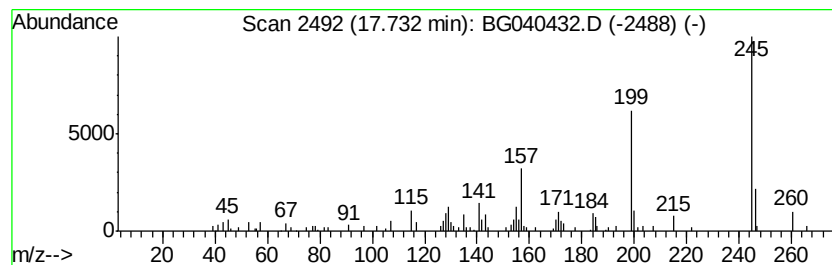
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 2-Nitrophenoxathin Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.73	2.40 ng	74582	Phenanthrene-d10	17.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Nitrophenoxathin	245	C12H7N03S	057106-95-3	53
2		Furo[3,2-c]quinoline, 2,3-dihydr...	245	C14H15N03	1000264-83-9	49
3		1H-Indene-4-acetic acid, 6-(1,1-...	260	C17H24O2	055591-05-4	43
4		Isothiourea, 2-methyl-1-(2,4-dim...	260	C15H20N2S	1000267-73-5	43
5		3-Pyridinemethanol, .alpha.-[3-...	260	C16H24N2O	1000337-80-3	38



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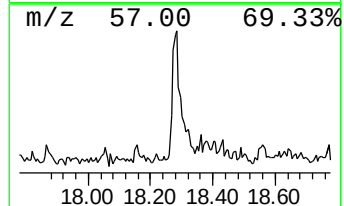
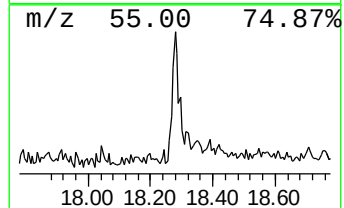
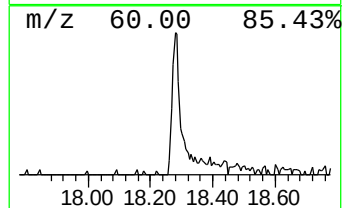
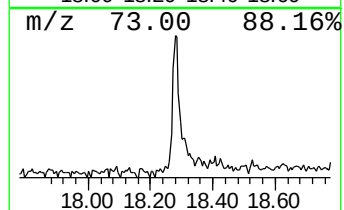
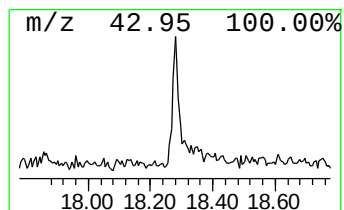
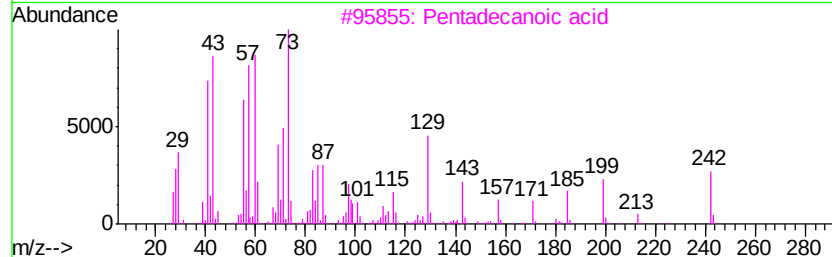
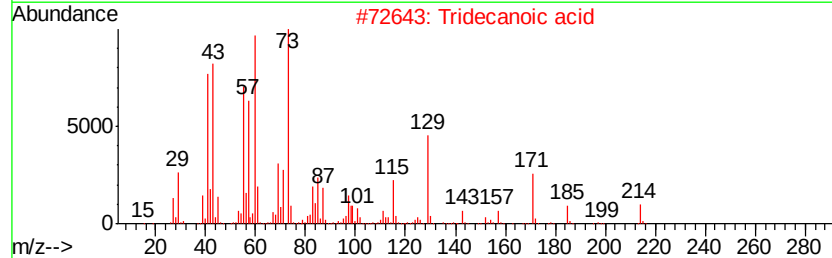
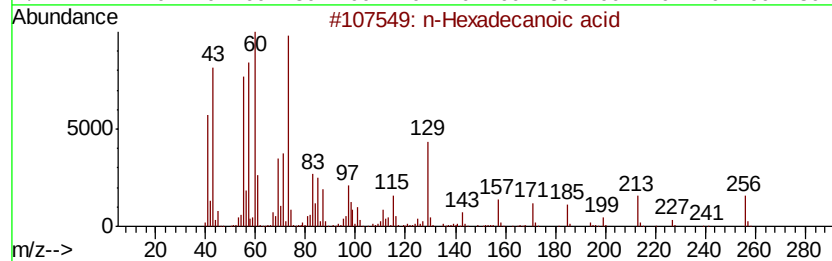
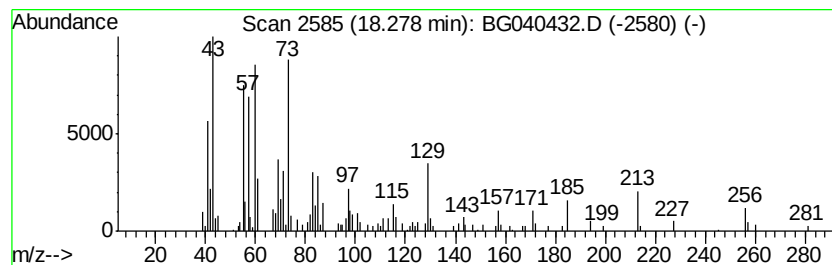
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.28	4.20 ng	130395	Phenanthrene-d10	17.42	
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	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



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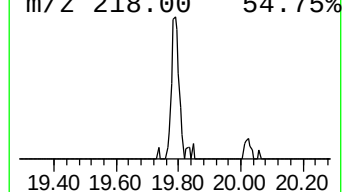
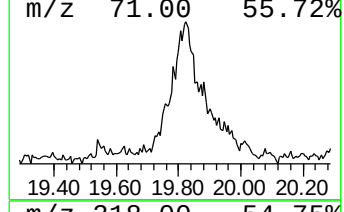
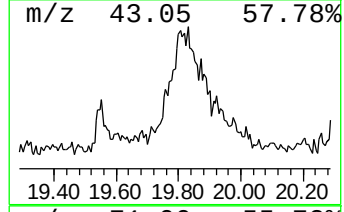
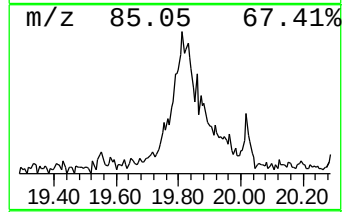
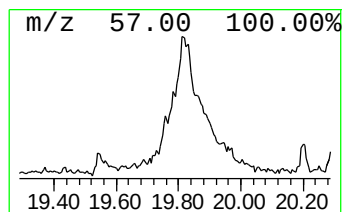
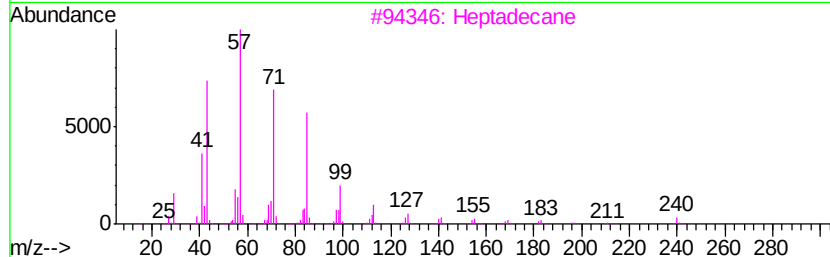
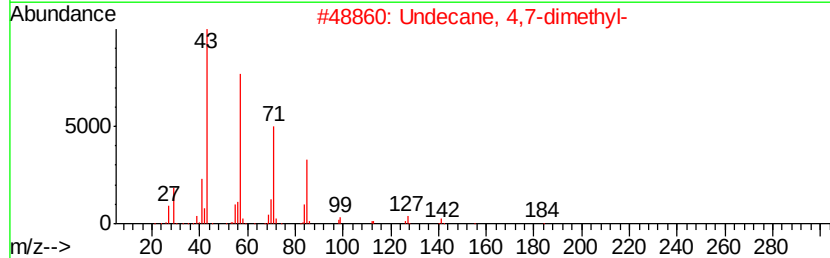
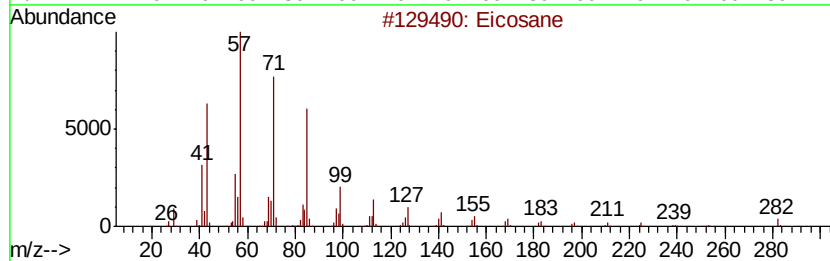
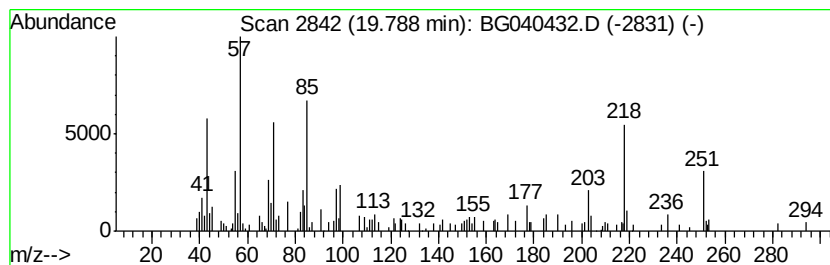
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Peak Number 6 unknown19.79 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	2.03 ng	83372	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	30
2		Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	27
3		Heptadecane	240	C17H36	000629-78-7	22
4		4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	22
5		Hexadecane	226	C16H34	000544-76-3	14



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ClientSampleId :
0237-COMP-CS-2-ELTRT

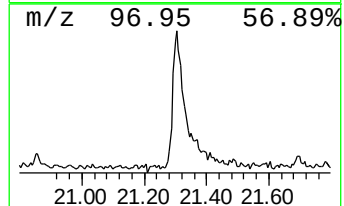
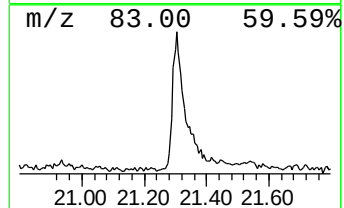
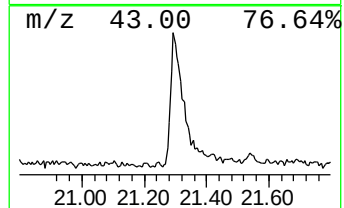
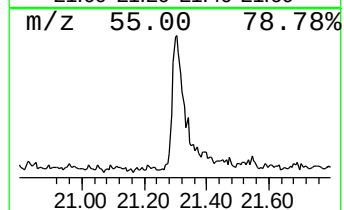
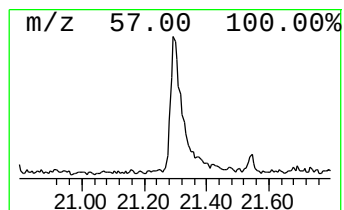
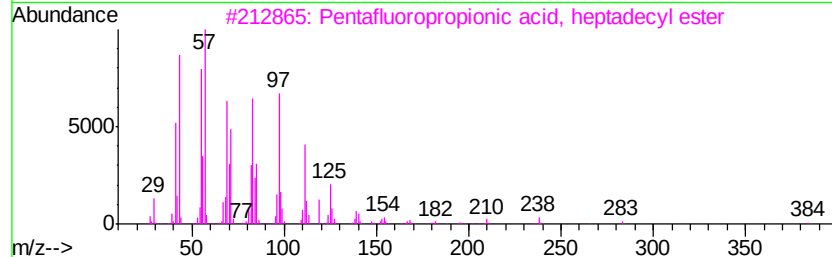
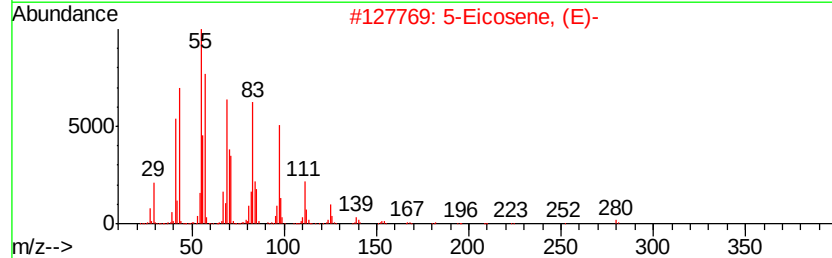
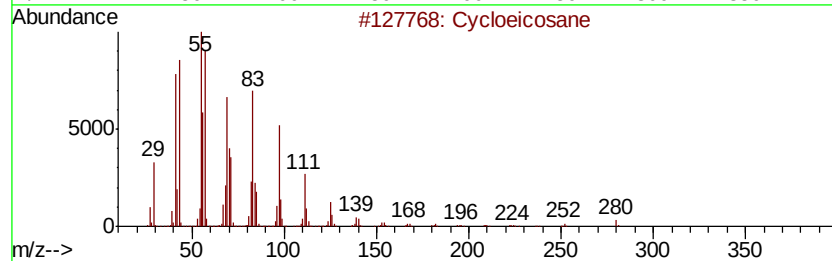
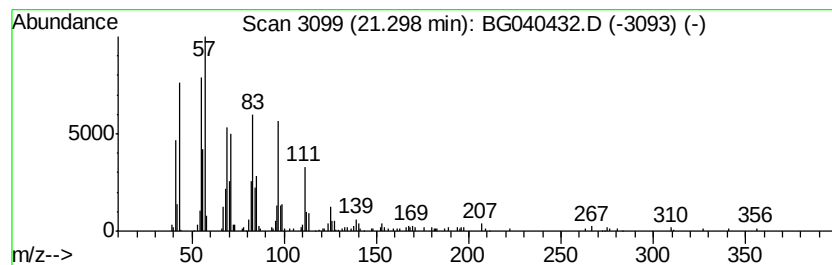
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cycloeicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	8.77 ng	360135	Chrysene-d12	21.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloeicosane	280	C20H40	000296-56-0	93
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	92
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4		1-Tricosene	322	C23H46	018835-32-0	91
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
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Acq On : 11 Apr 2019 3:45
Operator : JU/SJ
Sample : K2311-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

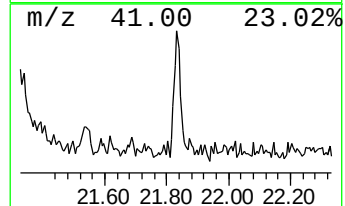
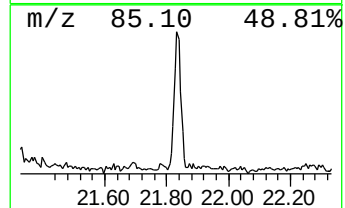
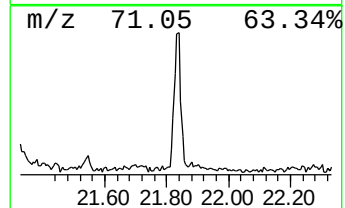
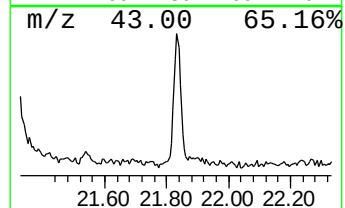
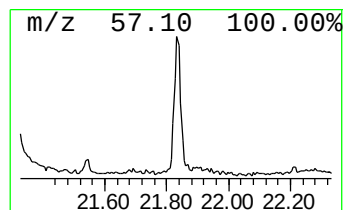
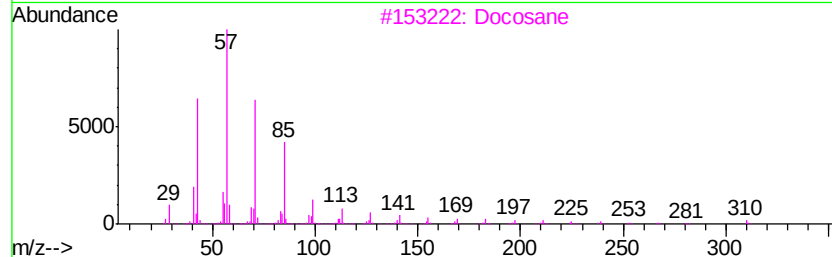
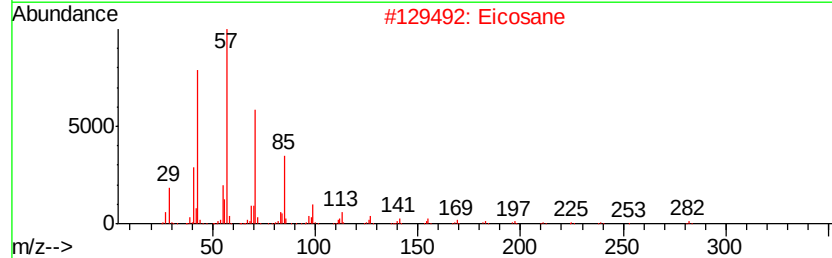
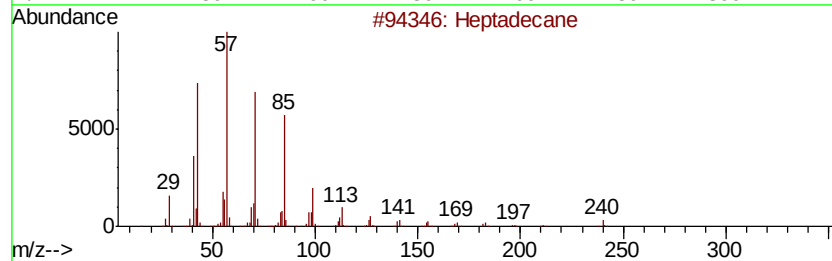
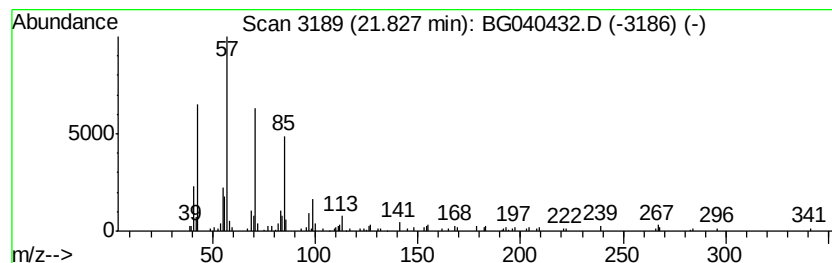
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
21.83	2.91 ng	119476	Chrysene-d12		21.69
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Eicosane	282	C20H42	000112-95-8	91
3	Docosane	310	C22H46	000629-97-0	91
4	Nonadecane	268	C19H40	000629-92-5	86
5	Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
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Sample : K2311-04
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ClientSampleId :
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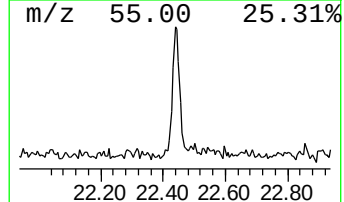
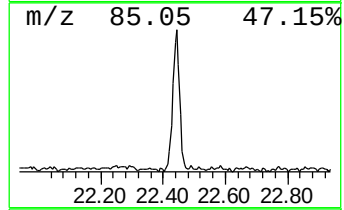
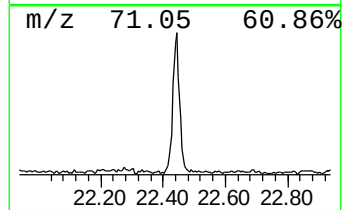
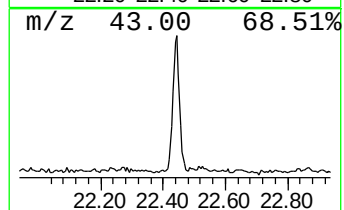
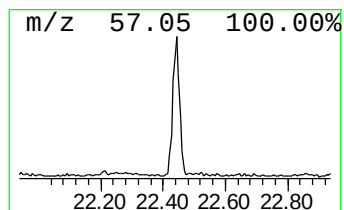
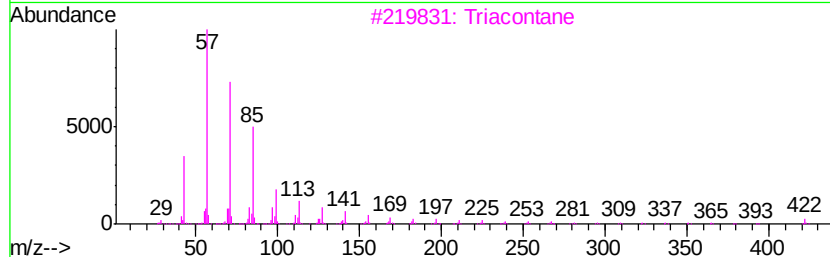
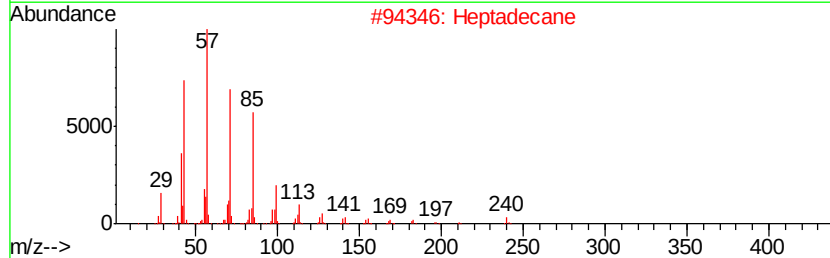
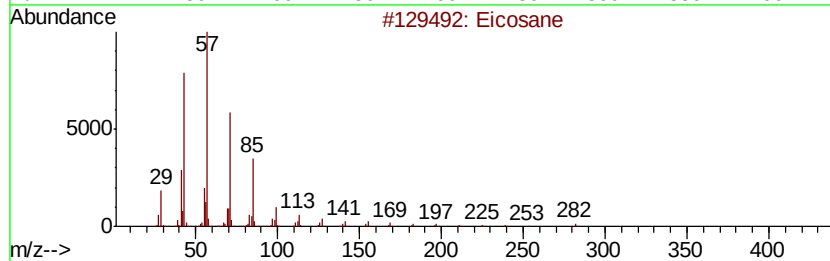
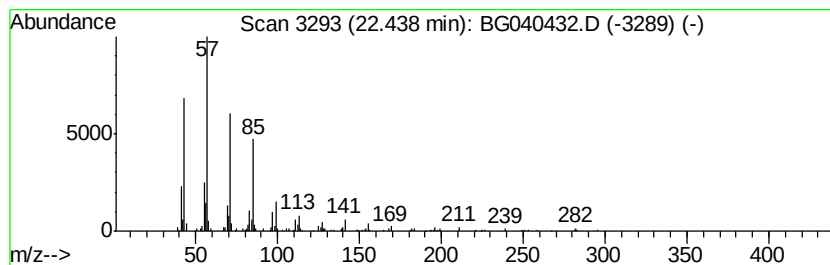
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.44	5.04 ng	206981	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heptadecane	240	C17H36	000629-78-7	90
3		Triacontane	422	C30H62	000638-68-6	90
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5		Octacosane	394	C28H58	000630-02-4	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
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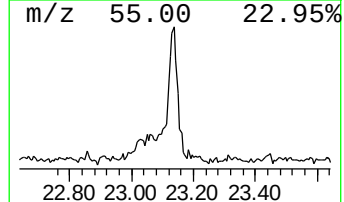
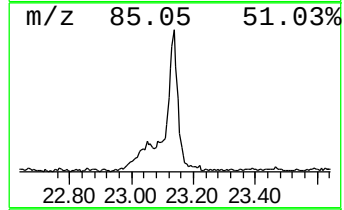
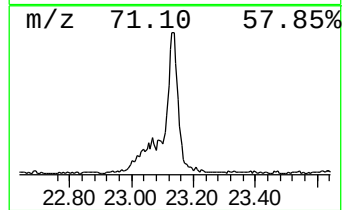
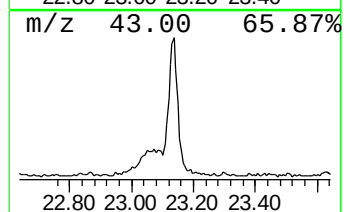
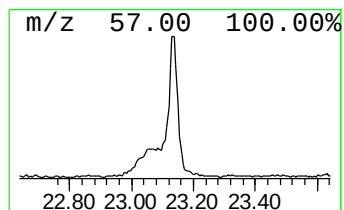
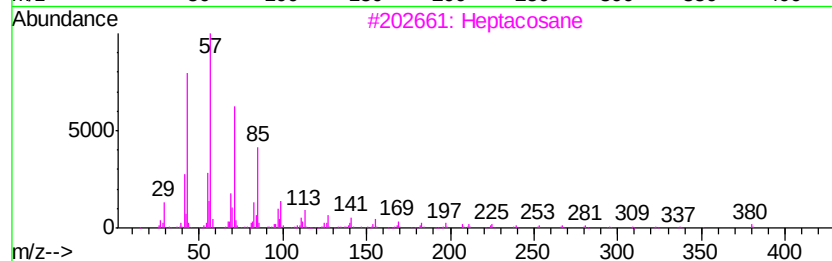
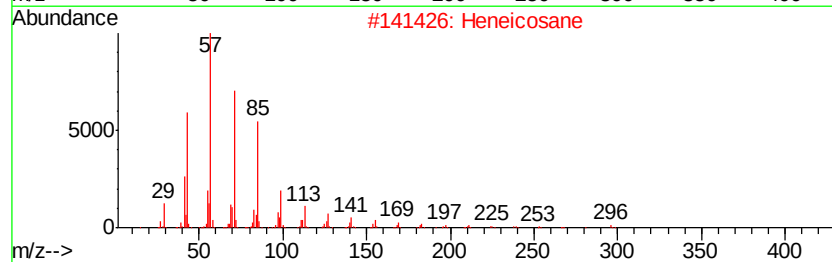
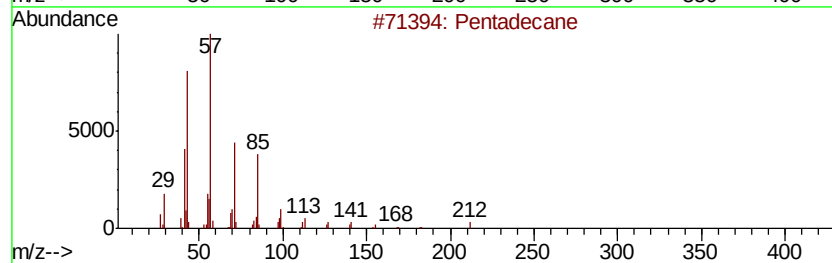
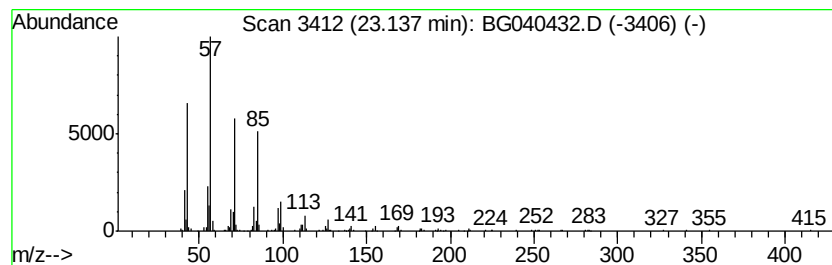
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TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 10 Pentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	10.22 ng	419703	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	87
2		Heneicosane	296	C21H44	000629-94-7	86
3		Heptacosane	380	C27H56	000593-49-7	86
4		Nonadecane	268	C19H40	000629-92-5	86
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
Data File : BG040432.D
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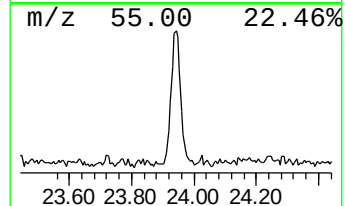
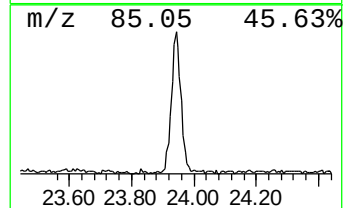
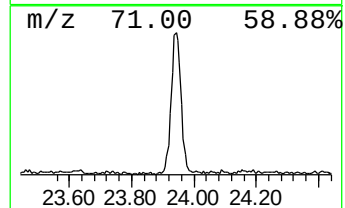
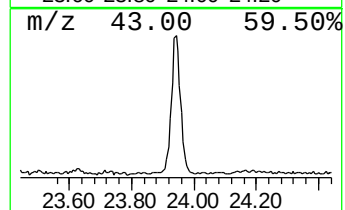
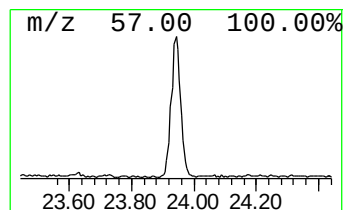
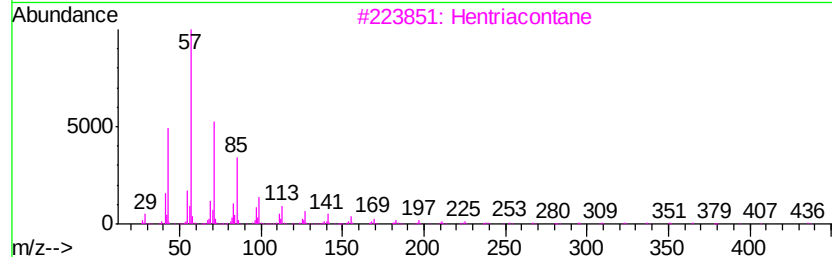
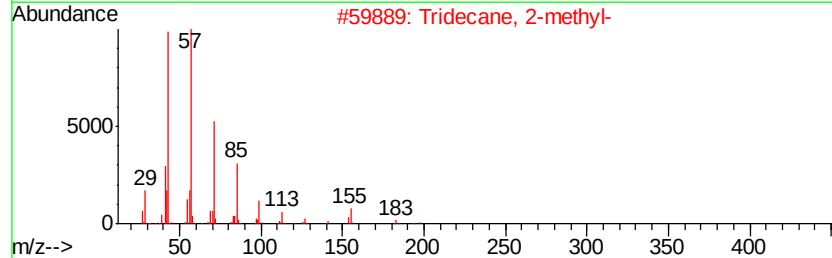
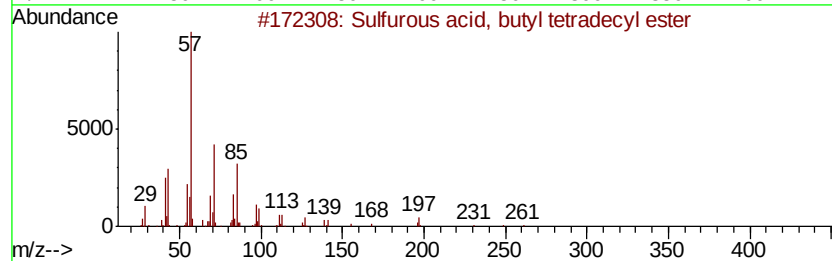
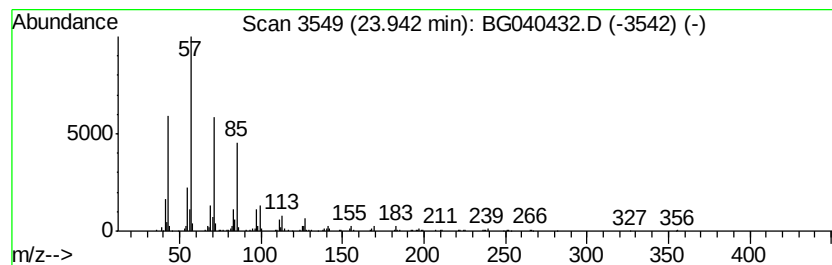
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Sulfurous acid, butyl tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.94	10.11 ng	388848	Perylene-d12	24.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	90
2		Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
3		Hentriacontane	437	C31H64	000630-04-6	80
4		Hexacosane	366	C26H54	000630-01-3	76
5		Eicosane	282	C20H42	000112-95-8	68



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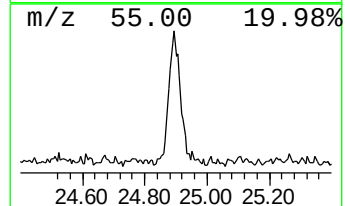
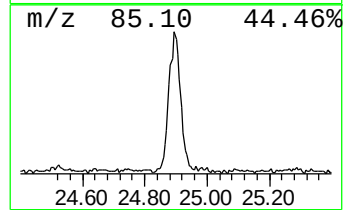
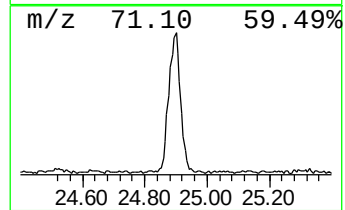
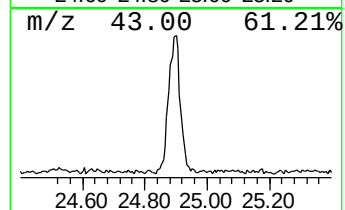
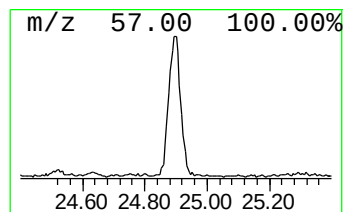
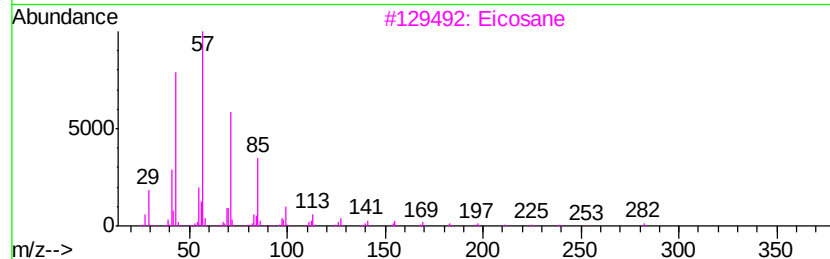
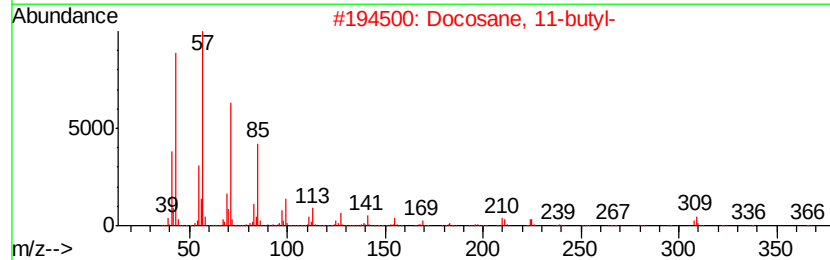
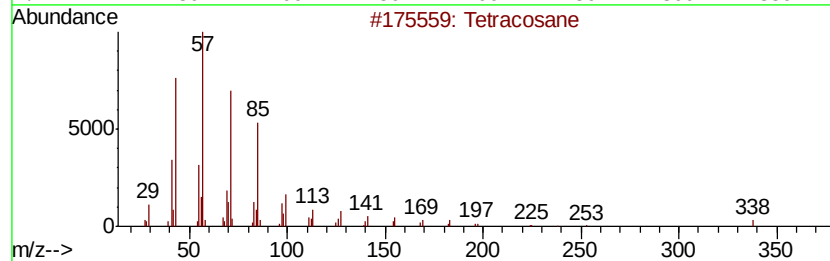
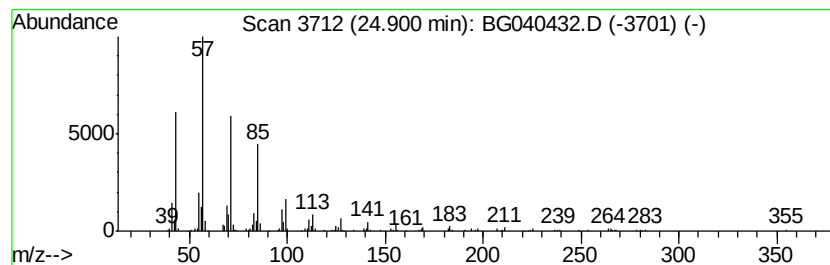
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TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 12 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.90	10.99 ng	422557	Perylene-d12	24.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
3		Eicosane	282	C20H42	000112-95-8	87
4		Heneicosane	296	C21H44	000629-94-7	83
5		Nonadecane	268	C19H40	000629-92-5	83



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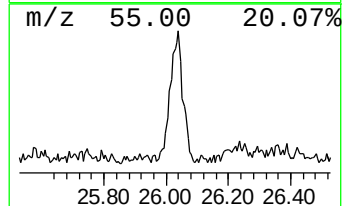
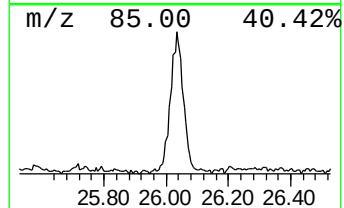
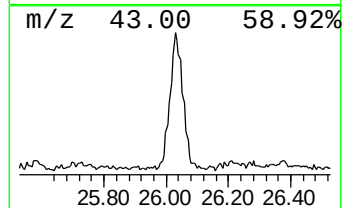
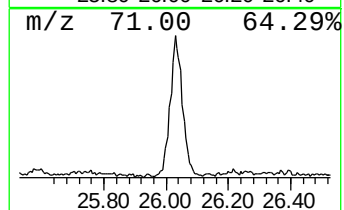
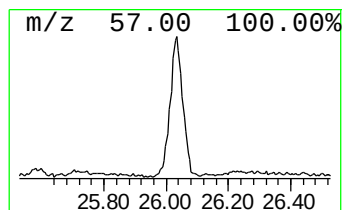
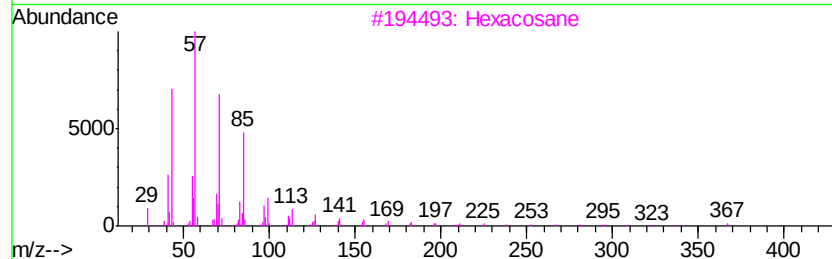
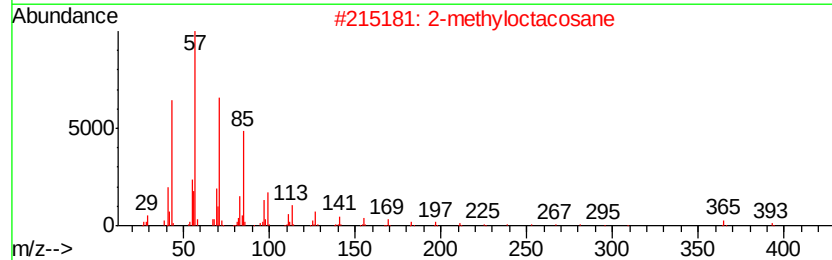
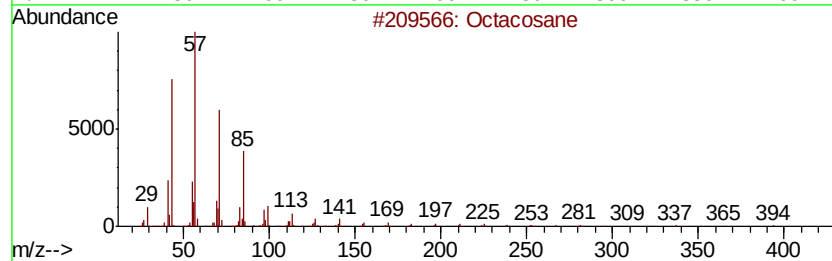
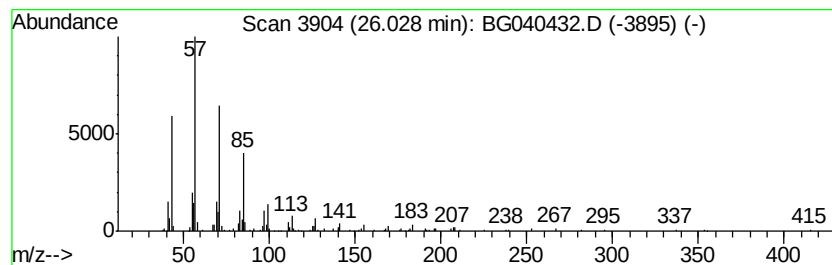
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.03	8.14 ng	313048	Perylene-d12	24.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
Data File : BG040432.D
Acq On : 11 Apr 2019 3:45
Operator : JU/SJ
Sample : K2311-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0237-COMP-CS-2-ELTRT

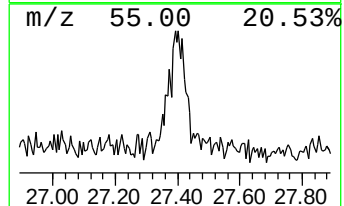
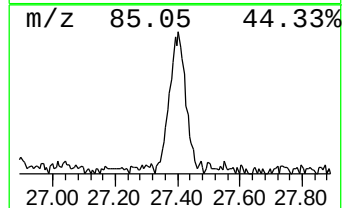
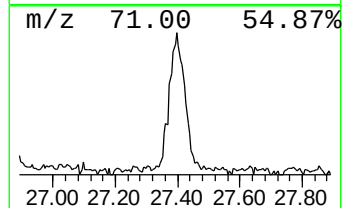
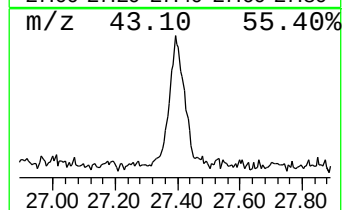
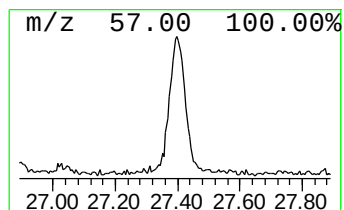
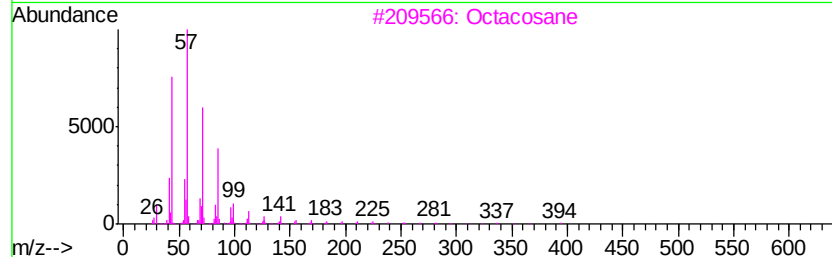
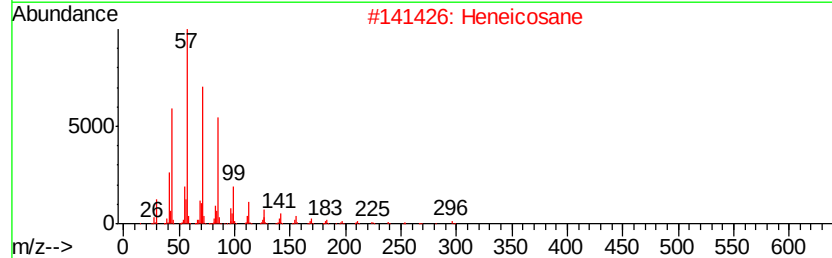
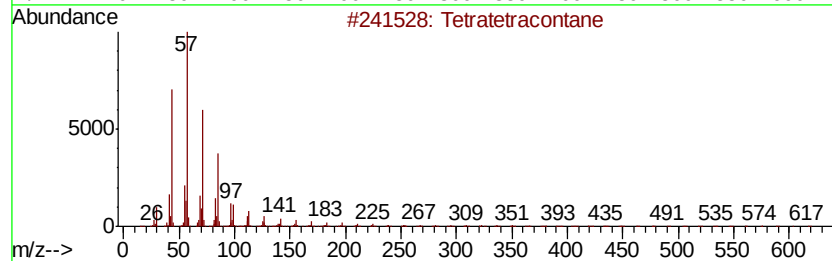
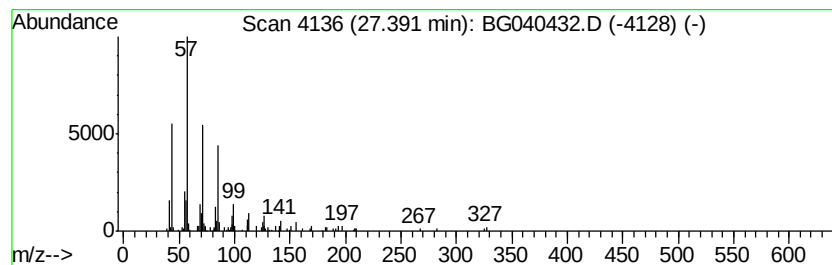
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.39	4.60 ng	176850	Perylene-d12	24.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Pentacosane	352	C25H52	000629-99-2	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041019\
Data File : BG040432.D
Acq On : 11 Apr 2019 3:45
Operator : JU/SJ
Sample : K2311-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0237-COMP-CS-2-ELTRT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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...	3.18	4.7	ng	53160	1	8.04	225839	20.0
unknown7.57	7.57	53.9	ng	609100	1	8.04	225839	20.0
2-Nitrophenoxathin	17.73	2.4	ng	74582	4	17.42	620915	20.0
n-Hexadecanoic acid	18.28	4.2	ng	130395	4	17.42	620915	20.0
unknown19.79	19.79	2.0	ng	83372	5	21.69	821332	20.0
Cycloeicosane	21.30	8.8	ng	360135	5	21.69	821332	20.0
Heptadecane	21.83	2.9	ng	119476	5	21.69	821332	20.0
Eicosane	22.44	5.0	ng	206981	5	21.69	821332	20.0
Pentadecane	23.14	10.2	ng	419703	5	21.69	821332	20.0
Sulfurous acid, b...	23.94	10.1	ng	388848	6	24.97	768926	20.0
Tetracosane	24.90	11.0	ng	422557	6	24.97	768926	20.0
Octacosane	26.03	8.1	ng	313048	6	24.97	768926	20.0
Tetratetracontane	27.39	4.6	ng	176850	6	24.97	768926	20.0