

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
 Data File : BG041713.D
 Acq On : 18 Jul 2019 17:09
 Operator : HP/JU
 Sample : K3835-46
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-8(4-6)

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-BG071519.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	3.200	14	19	31	rVB	326870	668233	11.84%	1.460%
2	5.145	345	350	360	rVB	32400	56993	1.01%	0.124%
3	5.609	422	429	445	rBV	1596996	2565514	45.47%	5.604%
4	7.195	691	699	711	rBV	1638995	2881310	51.07%	6.294%
5	7.577	756	764	773	rBV	1646088	2792697	49.50%	6.100%
6	8.047	836	844	852	rBV	388751	657863	11.66%	1.437%
7	8.370	891	899	912	rVB	1245358	2148540	38.08%	4.693%
8	9.199	1032	1040	1053	rBV	951236	1746421	30.95%	3.815%
9	10.850	1311	1321	1330	rBV	523789	947516	16.79%	2.070%
10	13.294	1730	1737	1747	rBV	2596003	4045556	71.70%	8.837%
11	14.005	1852	1858	1864	rVV	1099205	1602953	28.41%	3.501%
12	14.111	1867	1876	1889	rVB	299336	499317	8.85%	1.091%
13	14.634	1956	1965	1966	rBV	282025	353627	6.27%	0.772%
14	14.663	1966	1970	1976	rVB2	785735	1278402	22.66%	2.792%
15	14.927	2009	2015	2020	rVB2	82235	123158	2.18%	0.269%
16	14.998	2020	2027	2033	rVB3	66145	111445	1.98%	0.243%
17	15.603	2125	2130	2135	rBV2	48804	74568	1.32%	0.163%
18	16.044	2201	2205	2212	rVB2	72594	105215	1.86%	0.230%
19	16.144	2212	2222	2231	rBV	2120356	3280984	58.15%	7.167%
20	16.226	2231	2236	2244	rVB5	36866	71601	1.27%	0.156%
21	17.395	2426	2435	2445	rBV2	1101183	1698593	30.11%	3.710%
22	18.288	2581	2587	2597	rBV	175173	320061	5.67%	0.699%
23	20.004	2872	2879	2890	rBV	3942657	5642129	100.00%	12.324%
24	20.309	2926	2931	2940	rBV5	42741	101564	1.80%	0.222%
25	20.586	2974	2978	2983	rBV	147465	183509	3.25%	0.401%
26	21.120	3063	3069	3080	rVB	3397567	4536275	80.40%	9.909%
27	21.320	3097	3103	3122	rBV	248907	854027	15.14%	1.865%
28	21.649	3152	3159	3167	rBV	1145651	1882710	33.37%	4.112%
29	21.866	3192	3196	3202	rVB	55530	85878	1.52%	0.188%
30	22.477	3295	3300	3309	rBV3	82537	238307	4.22%	0.521%
31	23.171	3413	3418	3425	rVB2	92365	175792	3.12%	0.384%
32	23.365	3443	3451	3464	rVB	797234	1523761	27.01%	3.328%
33	23.982	3550	3556	3563	rBV2	95328	194457	3.45%	0.425%
34	24.839	3691	3702	3712	rBV	681808	1948078	34.53%	4.255%

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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

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35	24.933	3712	3718	3729	rVB2	76025	203149	3.60%	0.444%
36	26.073	3906	3912	3922	rVB2	60716	181149	3.21%	0.396%

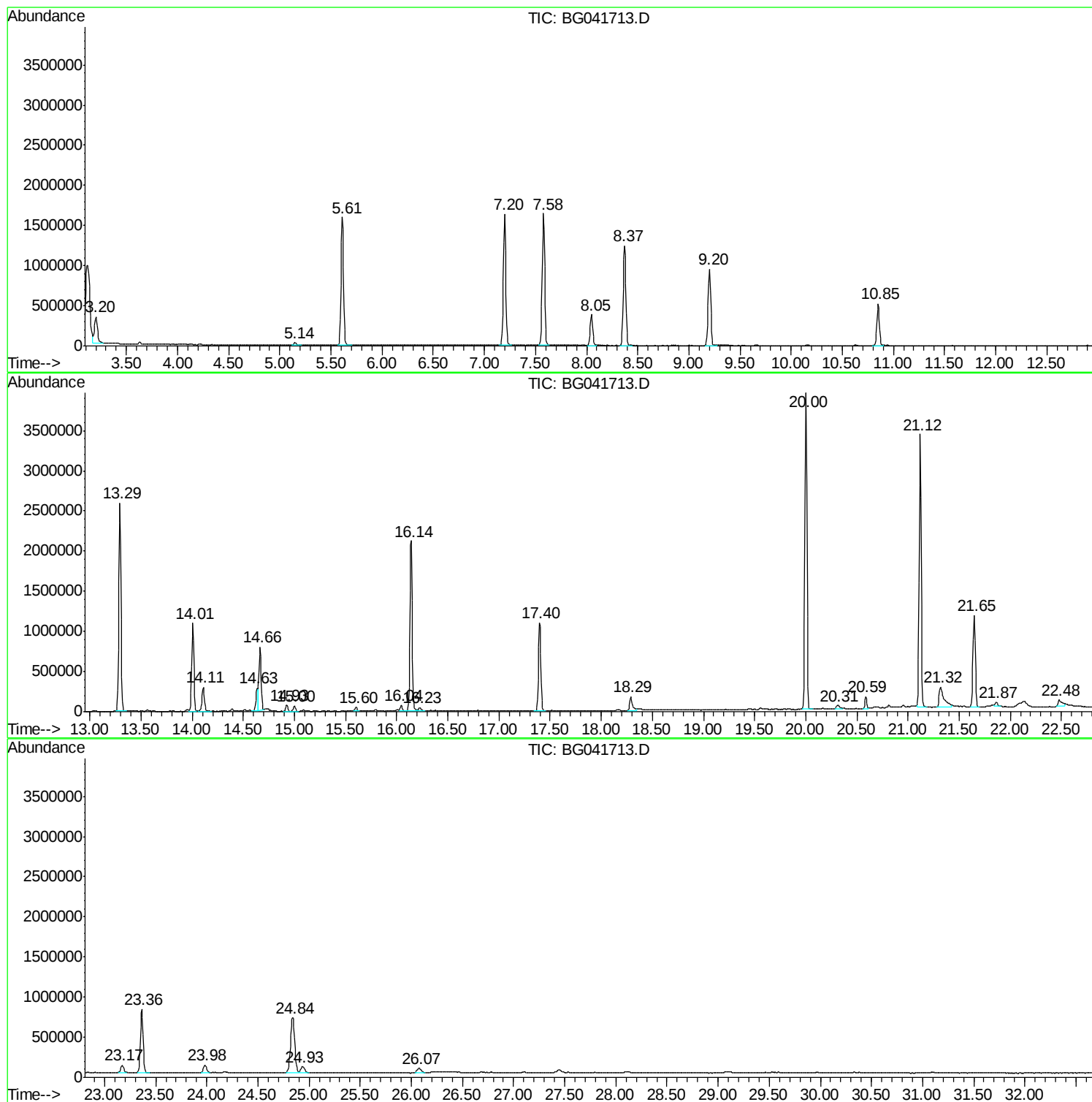
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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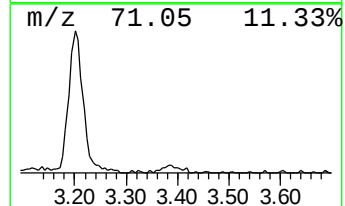
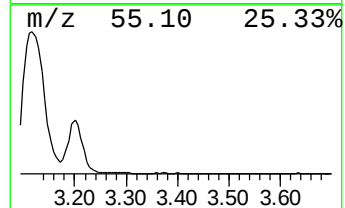
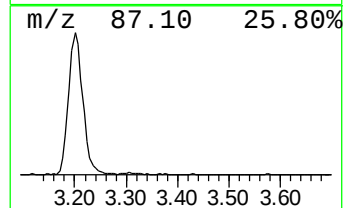
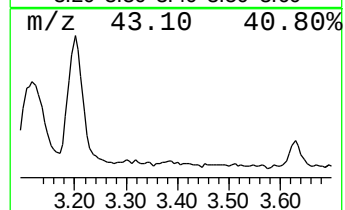
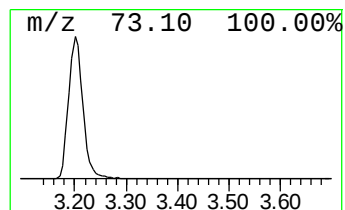
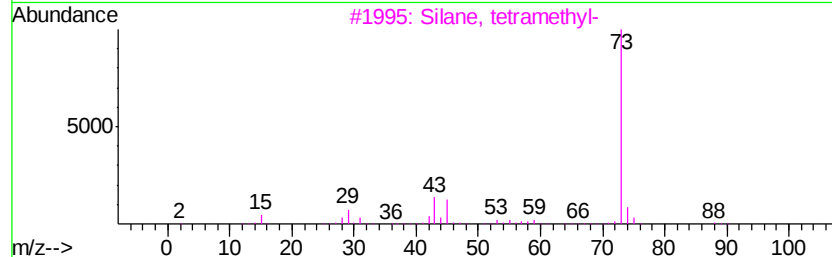
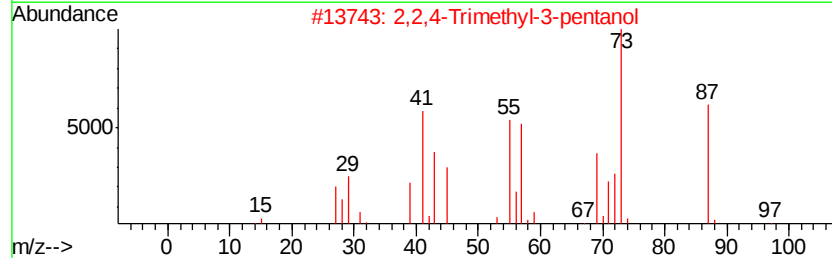
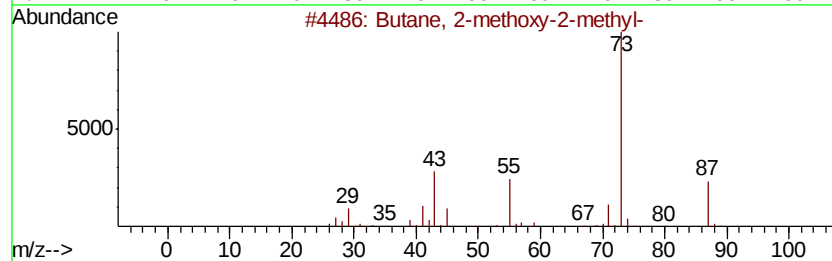
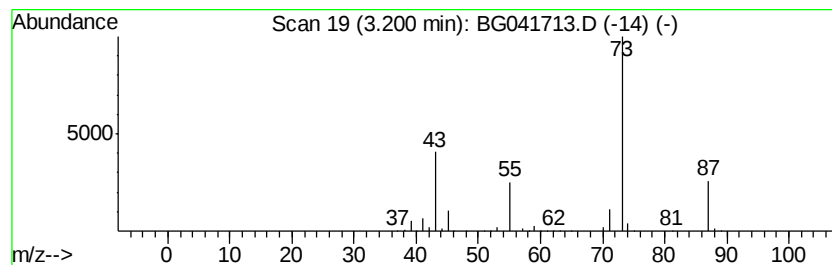
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG071519.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	20.32 ng	668233	1,4-Dichlorobenzene-d4	8.05

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	50
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		1,3-Dioxolane, 2-heptyl-	172	C10H20O2	004359-57-3	9



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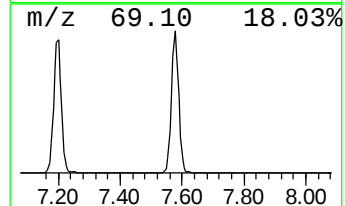
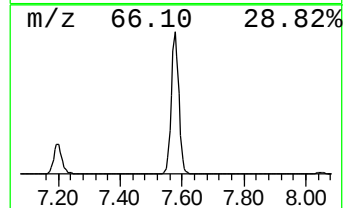
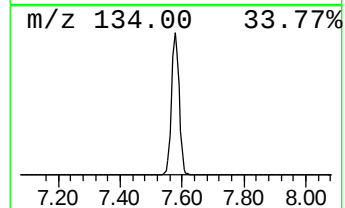
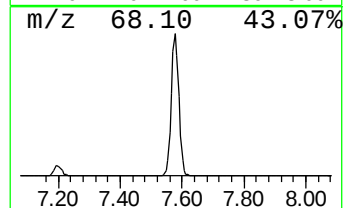
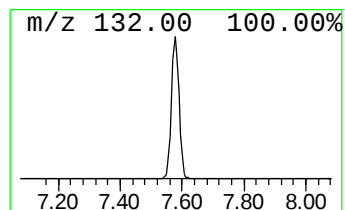
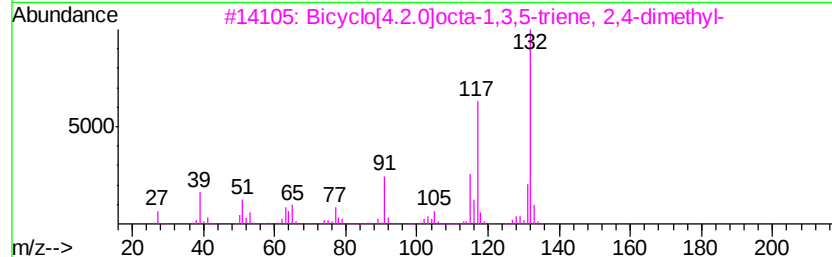
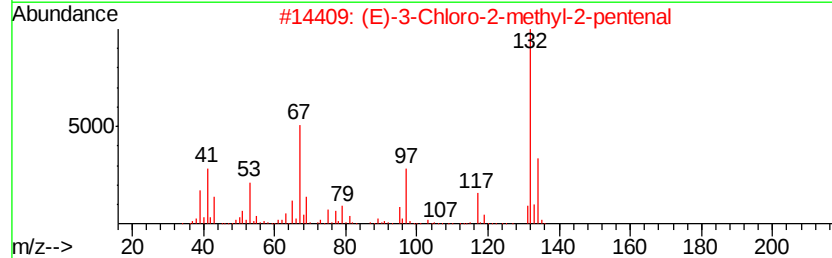
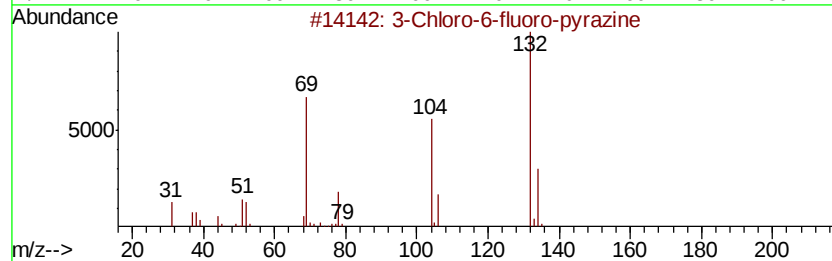
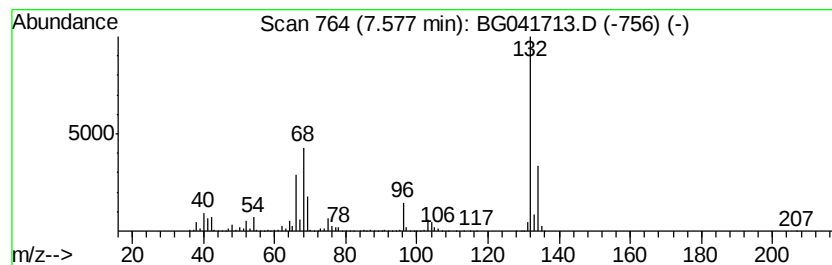
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Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	84.90 ng	2792700	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		Xenon	132	Xe	007440-63-3	9



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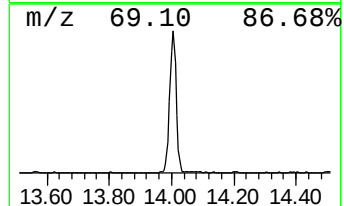
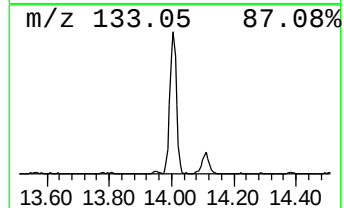
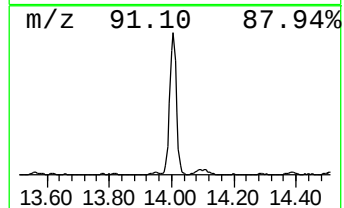
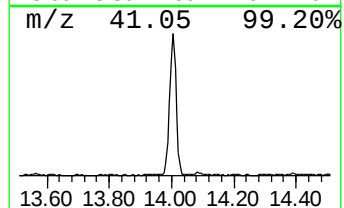
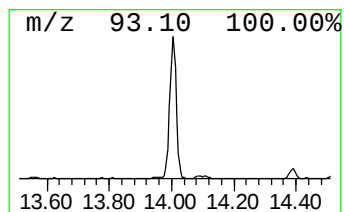
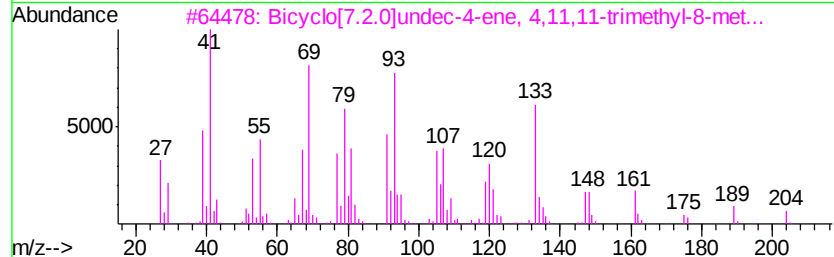
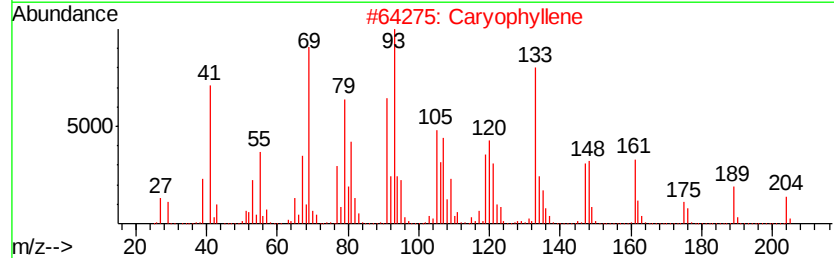
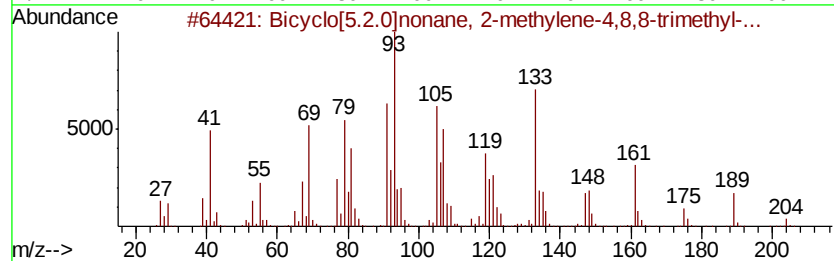
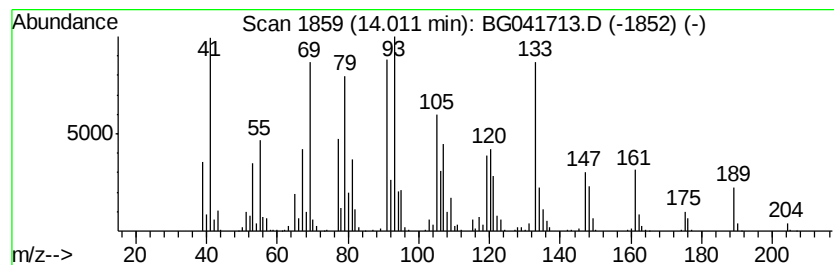
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Peak Number 4 Bicyclo[5.2.0]nonane, 2-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	25.08 ng	1602950	Acenaphthene-d10	14.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Bicyclo[5.2.0]nonane, 2-methylen...	204 C15H24	242794-76-9 93
2		Carvophyllene	204 C15H24	000087-44-5 93
3		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	000118-65-0 91
4		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204 C15H24	013877-93-5 70
5		Cyclohexane, 1,5-diethenyl-3-met...	162 C12H18	074742-35-1 46



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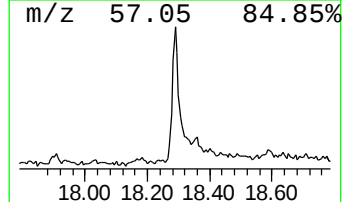
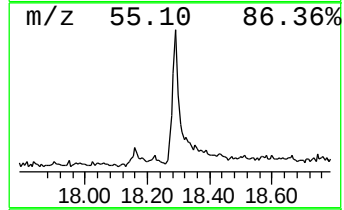
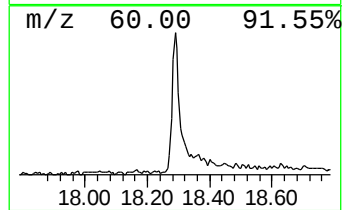
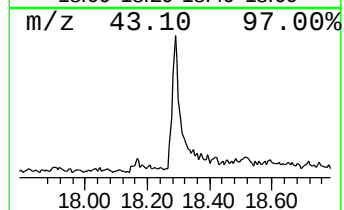
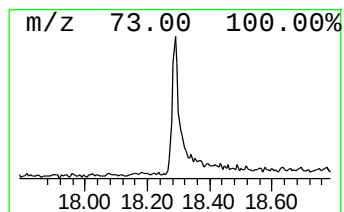
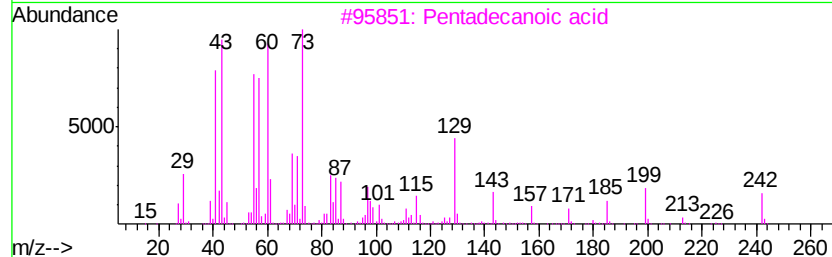
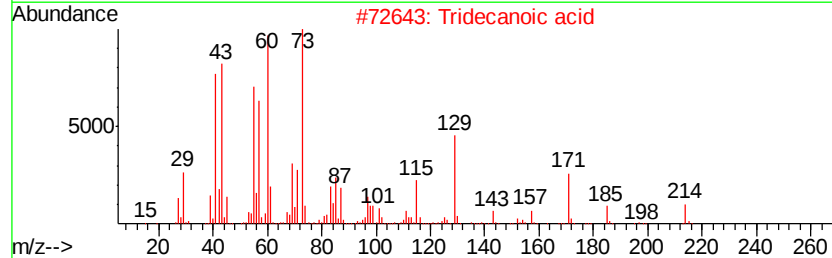
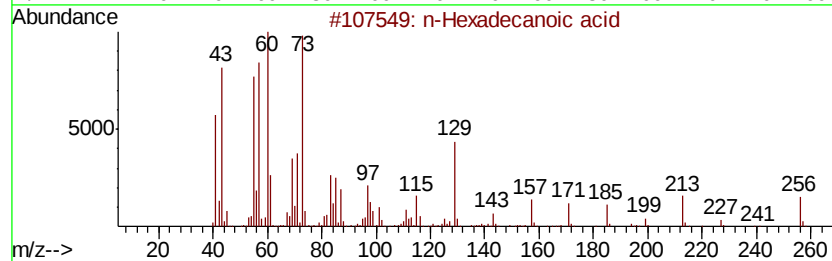
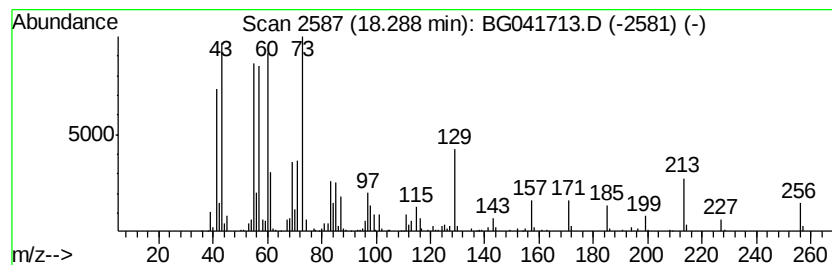
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	3.77 ng	320061	Phenanthrene-d10	17.40

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	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		n-Decanoic acid	172	C10H20O2	000334-48-5	60
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	53



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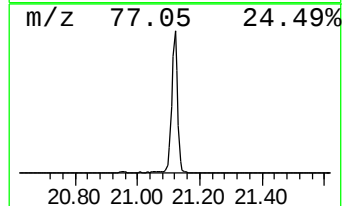
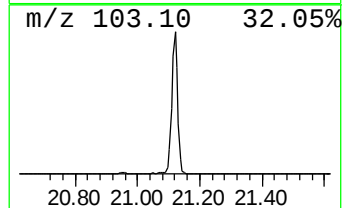
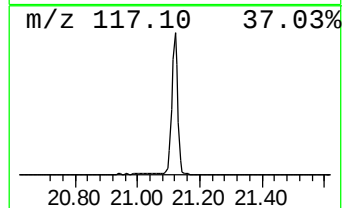
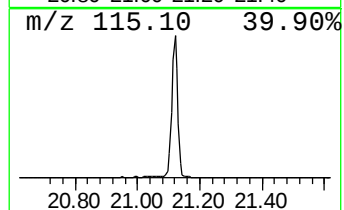
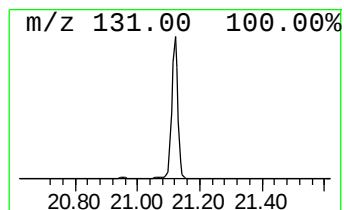
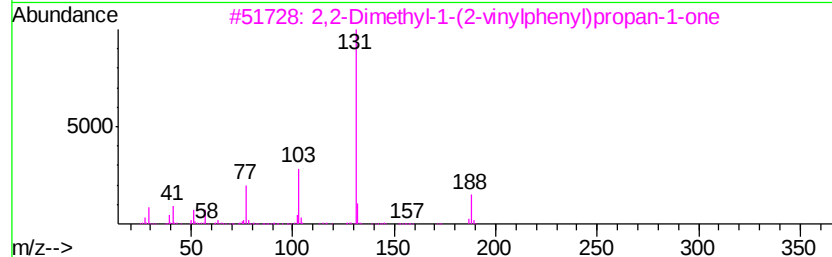
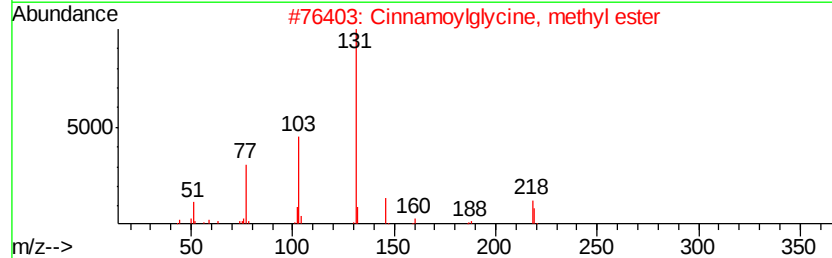
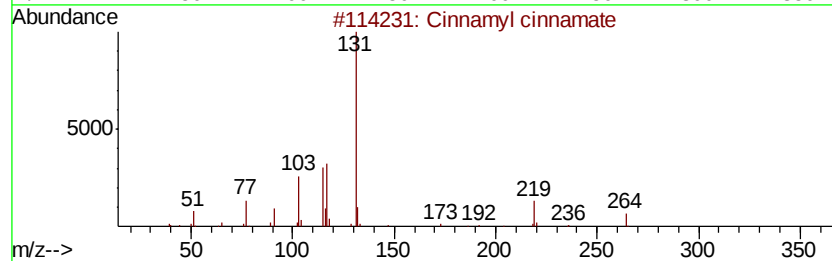
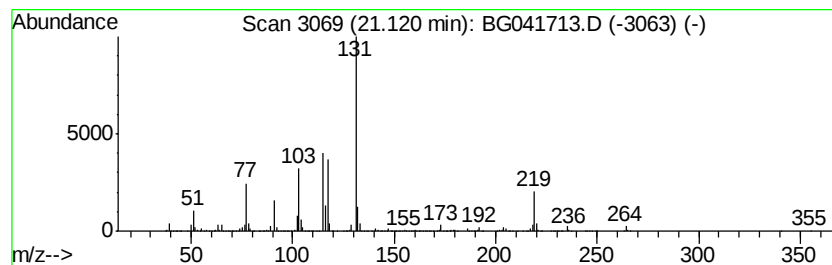
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Peak Number 6 Cinnamyl cinnamate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.12	48.19 ng	4536280	Chrysene-d12	21.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	86
2		Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	47
3		2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	46
4		Oxalic acid, monoamide monohydra...	323	C18H17N3O3	1000294-01-4	43
5		trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041713.D
Acq On : 18 Jul 2019 17:09
Operator : HP/JU
Sample : K3835-46
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-8(4-6)

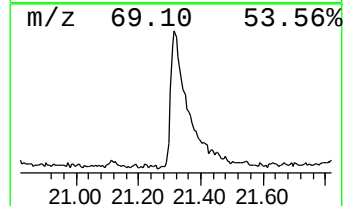
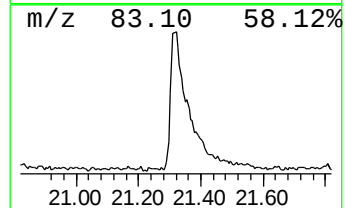
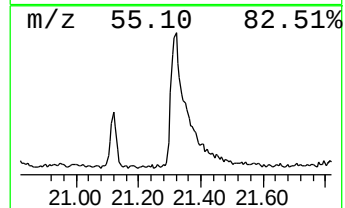
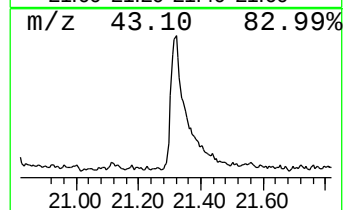
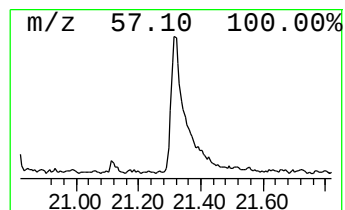
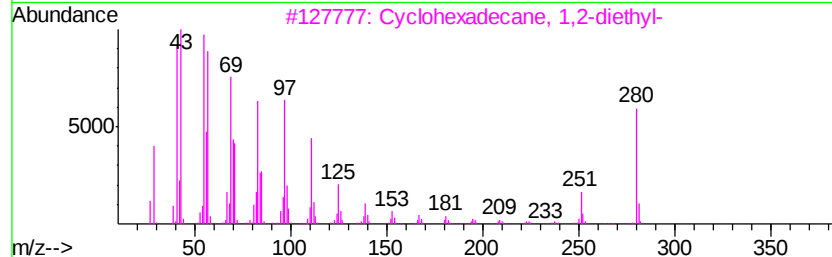
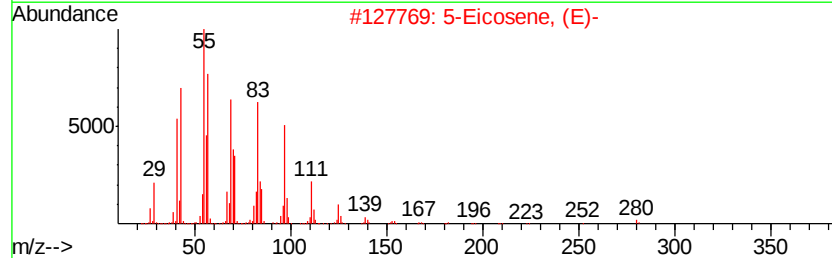
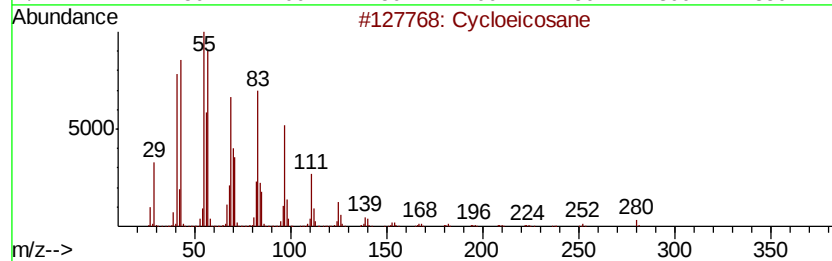
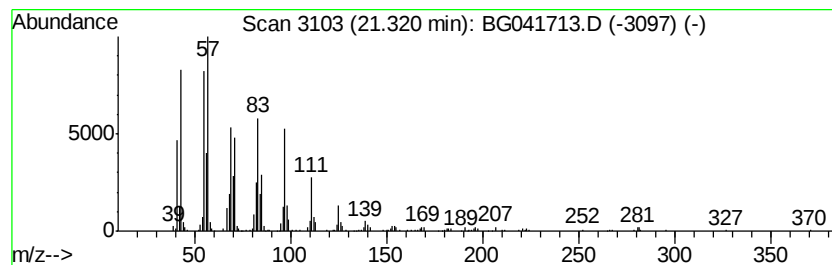
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cycloeicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	9.07 ng	854027	Chrysene-d12	21.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloeicosane	280	C20H40	000296-56-0	98
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
3		Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	97
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	97
5		Cyclotetracosane	336	C24H48	000297-03-0	95



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
 Data File : BG041713.D
 Acq On : 18 Jul 2019 17:09
 Operator : HP/JU
 Sample : K3835-46
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-8(4-6)

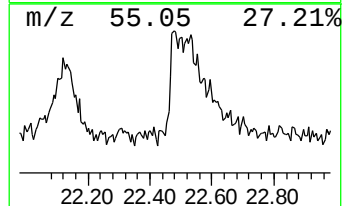
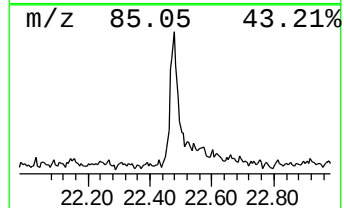
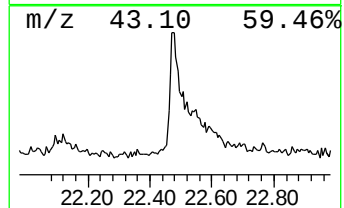
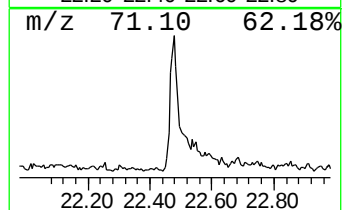
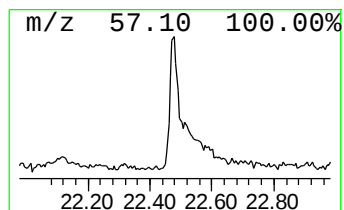
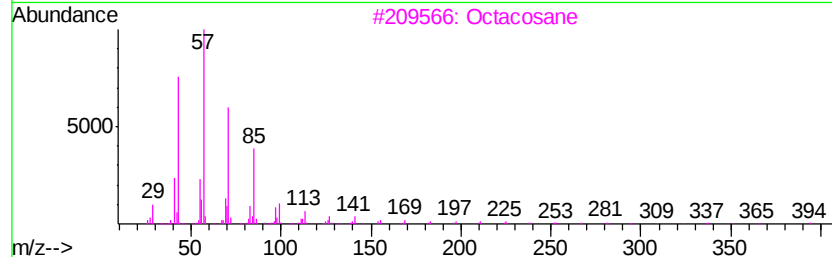
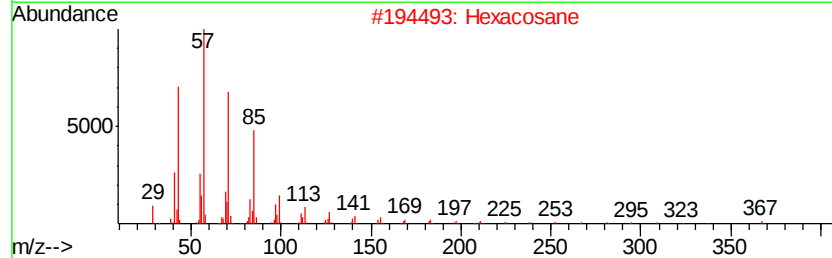
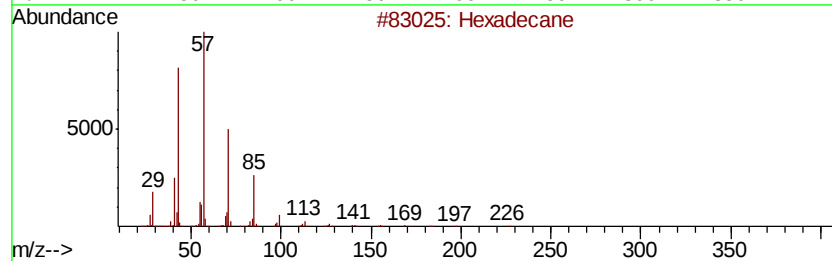
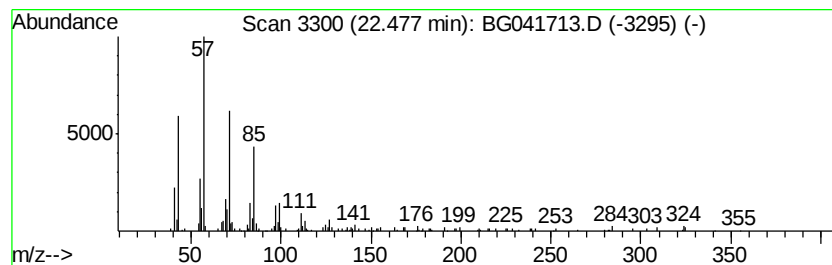
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	2.53 ng	238307	Chrysene-d12	21.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Hexacosane	366	C26H54	000630-01-3	90
3		Octacosane	394	C28H58	000630-02-4	87
4		Tetracosane	338	C24H50	000646-31-1	74
5		Nonadecane	268	C19H40	000629-92-5	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
 Data File : BG041713.D
 Acq On : 18 Jul 2019 17:09
 Operator : HP/JU
 Sample : K3835-46
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-8(4-6)

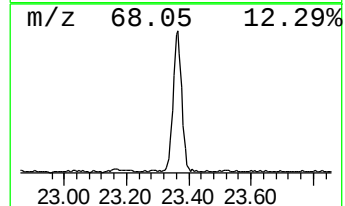
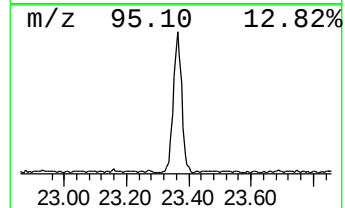
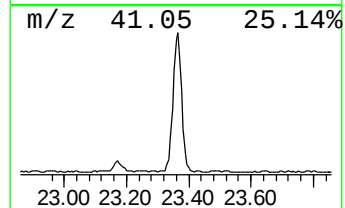
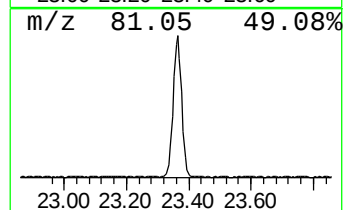
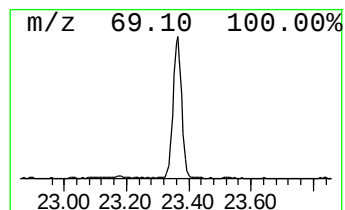
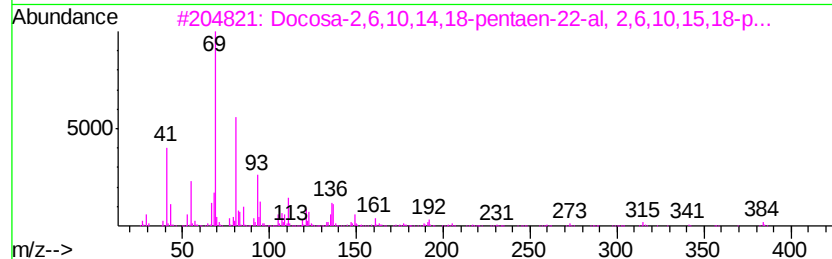
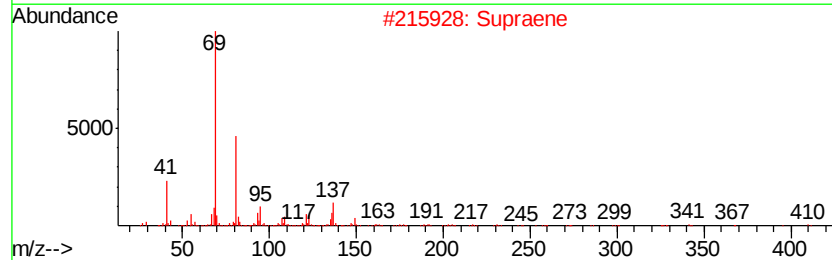
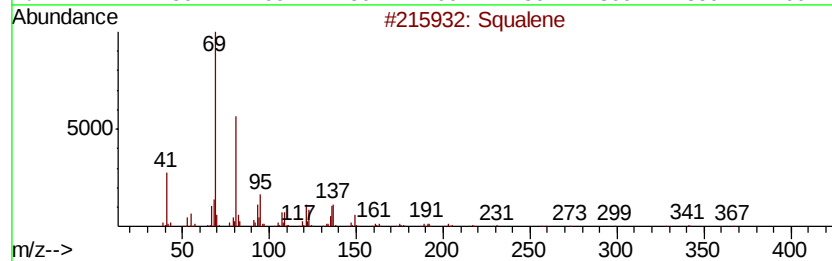
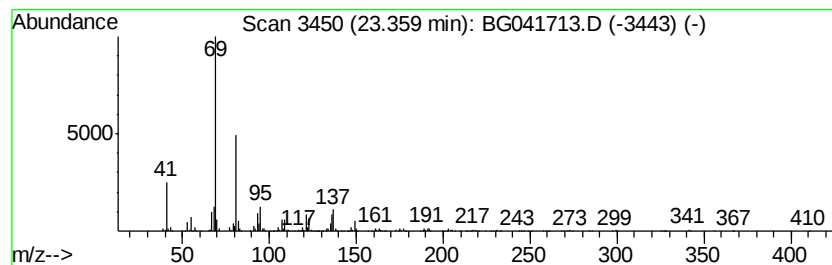
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	15.64 ng	1523760	Perylene-d12	24.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	94
2		Supraene	410	C30H50	007683-64-9	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041713.D
Acq On : 18 Jul 2019 17:09
Operator : HP/JU
Sample : K3835-46
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-8(4-6)

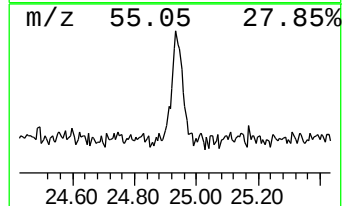
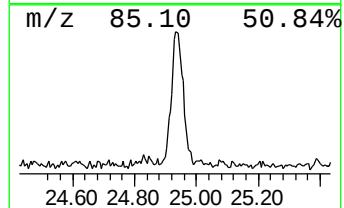
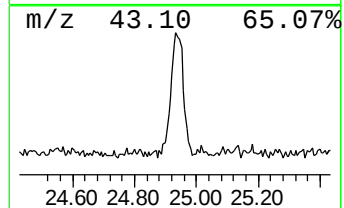
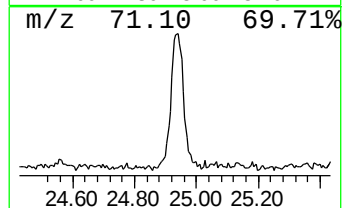
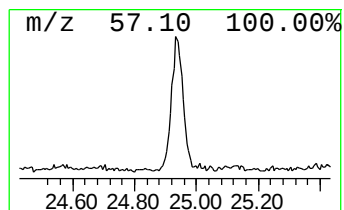
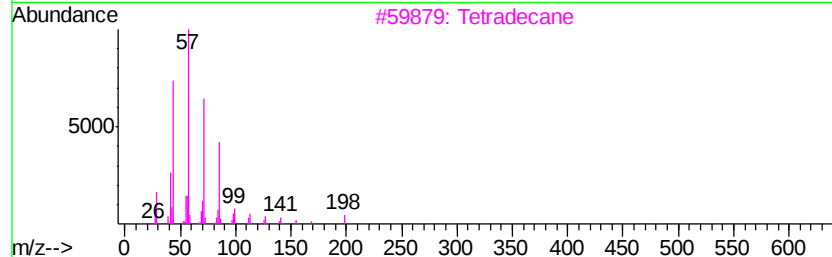
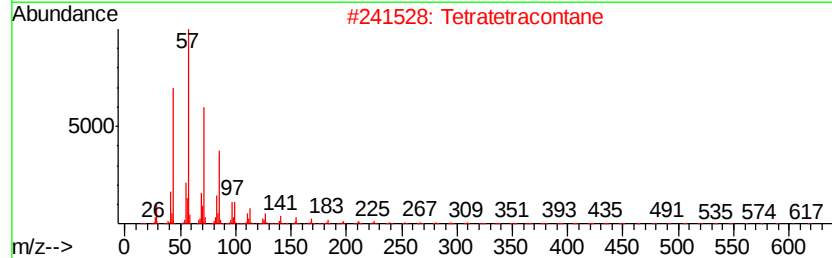
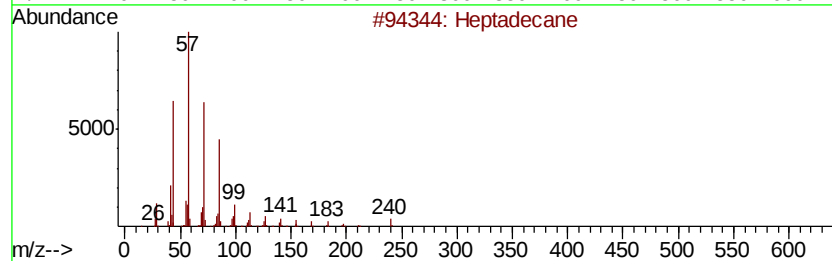
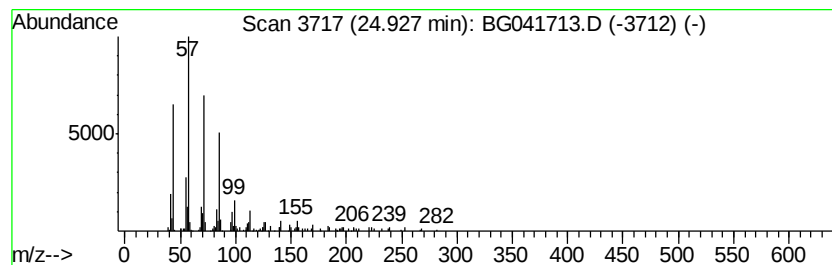
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.93	2.09 ng	203149	Perylene-d12	24.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	86
2		Tetratetracontane	619	C44H90	007098-22-8	86
3		Tetradecane	198	C14H30	000629-59-4	80
4		Heptacosane	380	C27H56	000593-49-7	80
5		Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071819\
Data File : BG041713.D
Acq On : 18 Jul 2019 17:09
Operator : HP/JU
Sample : K3835-46
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-8(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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...	3.20	20.3	ng	668233	1	8.05	657863	20.0
unknown7.58	7.58	84.9	ng	2792700	1	8.05	657863	20.0
Bicyclo[5.2.0]non...	14.01	25.1	ng	1602950	3	14.66	1278400	20.0
n-Hexadecanoic acid	18.29	3.8	ng	320061	4	17.40	1698590	20.0
Cinnamyl cinnamate	21.12	48.2	ng	4536280	5	21.65	1882710	20.0
Cycloeicosane	21.32	9.1	ng	854027	5	21.65	1882710	20.0
Hexadecane	22.48	2.5	ng	238307	5	21.65	1882710	20.0
Squalene	23.36	15.6	ng	1523760	6	24.84	1948080	20.0
Heptadecane	24.93	2.1	ng	203149	6	24.84	1948080	20.0