

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
 Data File : BG033956.D
 Acq On : 24 Apr 2018 16:15
 Operator : SJ/JU
 Sample : J2471-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MH-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:\HPCHEM1\BNA_G\METHODS\8270-BG041918.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	4.992	284	290	296	rVB	48334	72833	1.15%	0.237%
2	5.438	360	366	373	rBV	727549	1131736	17.83%	3.677%
3	5.515	373	379	388	rVB	61529	150073	2.36%	0.488%
4	6.995	624	631	639	rBV	464090	765266	12.06%	2.486%
5	7.365	685	694	702	rBV	1264787	2167667	34.15%	7.042%
6	7.829	762	773	781	rBV	265399	475474	7.49%	1.545%
7	8.147	819	827	834	rBV	1105256	1877628	29.58%	6.100%
8	8.211	834	838	855	rVB3	40376	88834	1.40%	0.289%
9	8.975	953	968	978	rBV	910732	1648508	25.97%	5.356%
10	10.027	1141	1147	1155	rVB2	51892	95775	1.51%	0.311%
11	10.609	1238	1246	1252	rBV	355909	636959	10.03%	2.069%
12	13.082	1656	1667	1676	rVB	2387377	3682396	58.01%	11.963%
13	13.916	1804	1809	1814	rBV	58426	88698	1.40%	0.288%
14	14.457	1893	1901	1908	rBV2	542753	895095	14.10%	2.908%
15	15.209	2024	2029	2034	rBV	52122	78177	1.23%	0.254%
16	15.503	2075	2079	2085	rVB	50843	72449	1.14%	0.235%
17	15.697	2107	2112	2116	rBV	57580	81253	1.28%	0.264%
18	15.949	2148	2155	2163	rBV2	2091365	3160724	49.79%	10.269%
19	16.131	2181	2186	2193	rVV	122376	187741	2.96%	0.610%
20	16.196	2194	2197	2206	rVB	47051	79785	1.26%	0.259%
21	16.478	2239	2245	2253	rBV	57322	91291	1.44%	0.297%
22	17.207	2362	2369	2379	rVB2	733294	1134681	17.87%	3.686%
23	18.129	2520	2526	2535	rBV	608687	930999	14.67%	3.025%
24	19.287	2719	2723	2729	rBV2	76426	108360	1.71%	0.352%
25	19.410	2739	2744	2759	rVB	397298	575337	9.06%	1.869%
26	19.651	2782	2785	2796	rVB2	42888	84678	1.33%	0.275%
27	19.851	2812	2819	2824	rBV	4642908	6348065	100.00%	20.624%
28	20.650	2951	2955	2964	rBV	176462	221086	3.48%	0.718%
29	21.155	3036	3041	3049	rBV2	205355	298505	4.70%	0.970%
30	21.466	3087	3094	3102	rBV	938330	1467601	23.12%	4.768%
31	23.129	3371	3377	3384	rBV	135341	247518	3.90%	0.804%
32	24.516	3603	3613	3626	rVB2	535677	1471851	23.19%	4.782%
33	26.214	3894	3902	3911	rBV2	29644	93913	1.48%	0.305%
34	26.637	3967	3974	3986	rBV10	61100	194055	3.06%	0.630%

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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 >
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35	29.604	4470	4479	4489	rvB10	20562	75490	1.19%	0.245%
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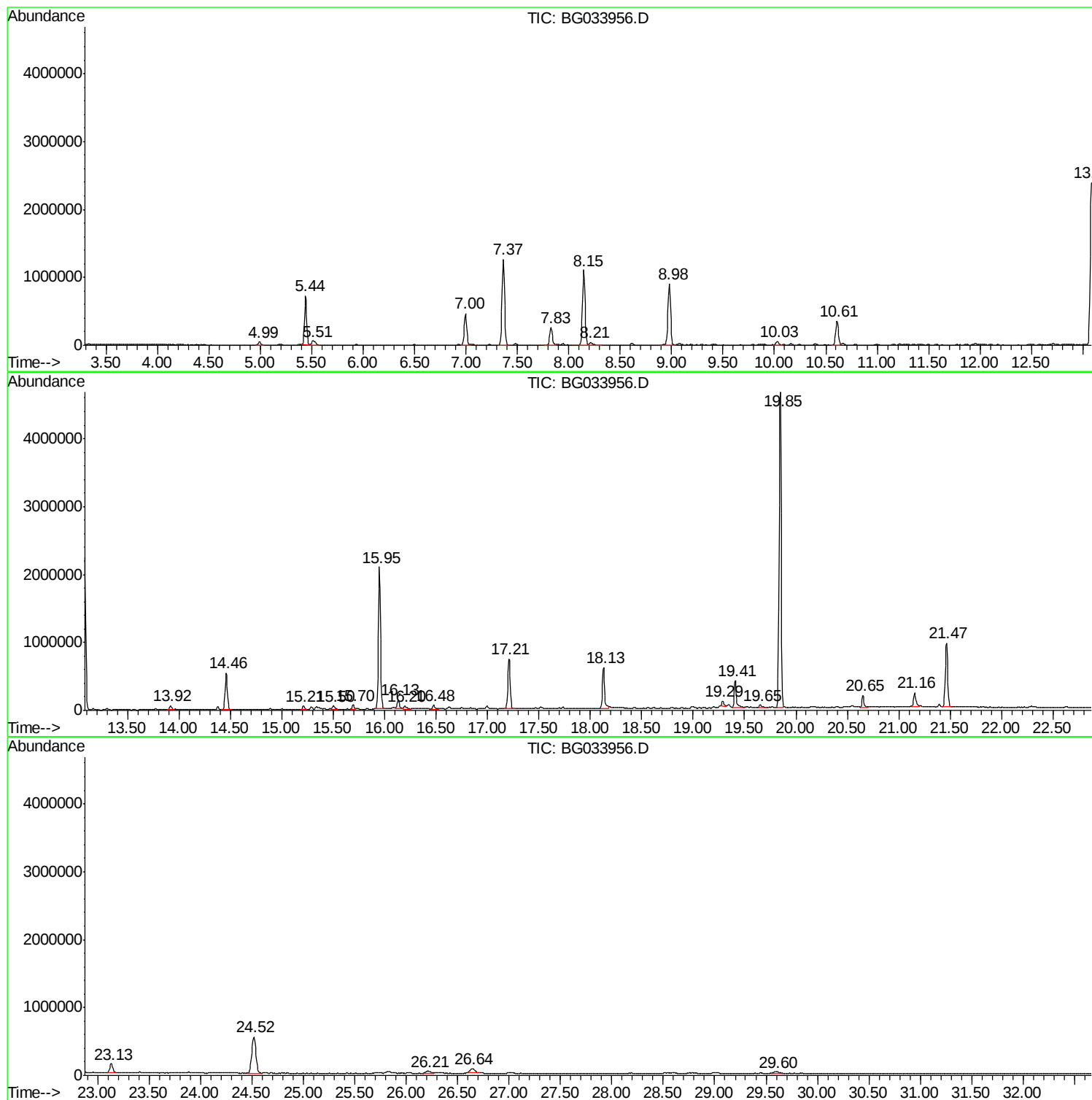
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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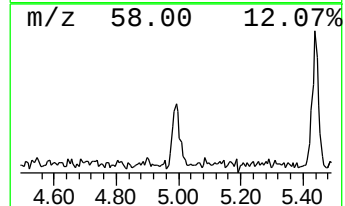
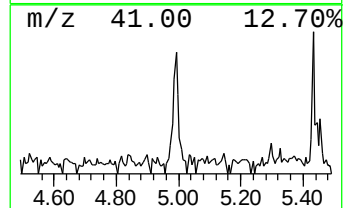
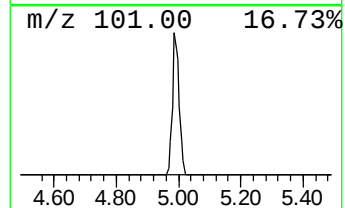
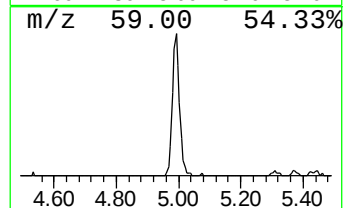
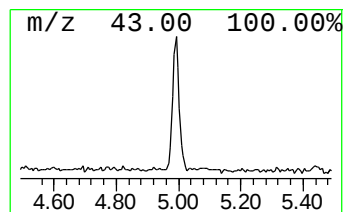
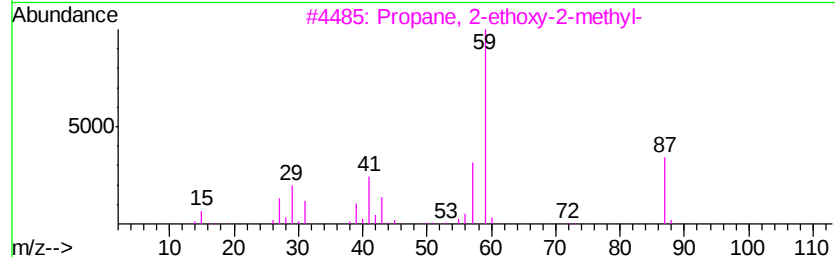
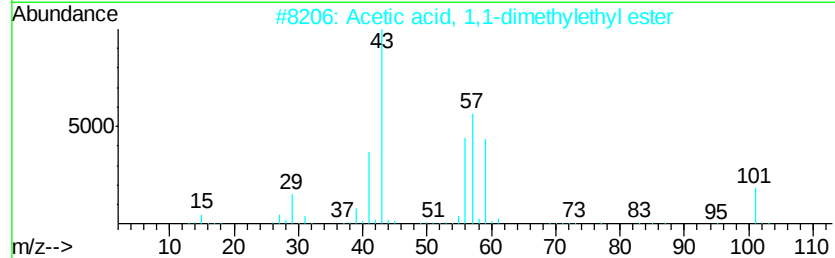
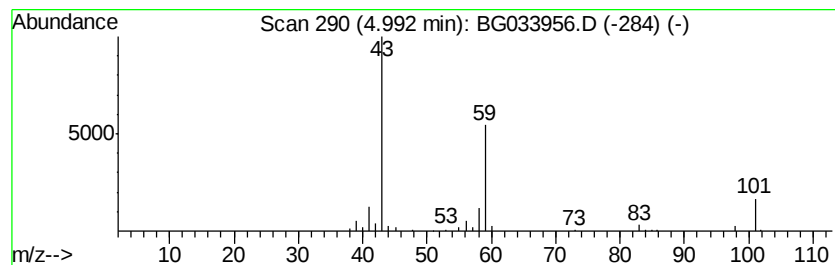
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	3.06 ng	72833	1,4-Dichlorobenzene-d4	7.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	32
4			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



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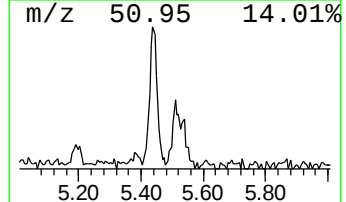
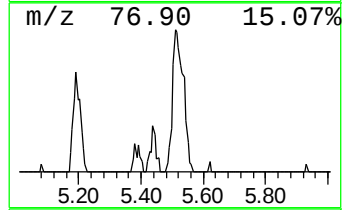
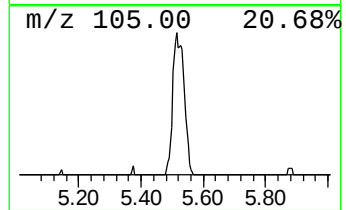
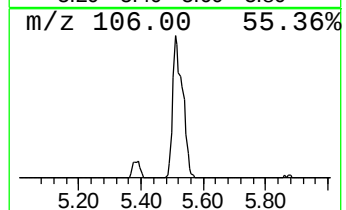
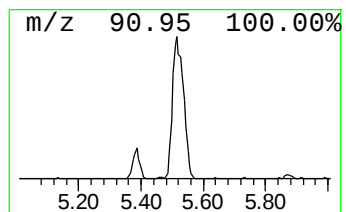
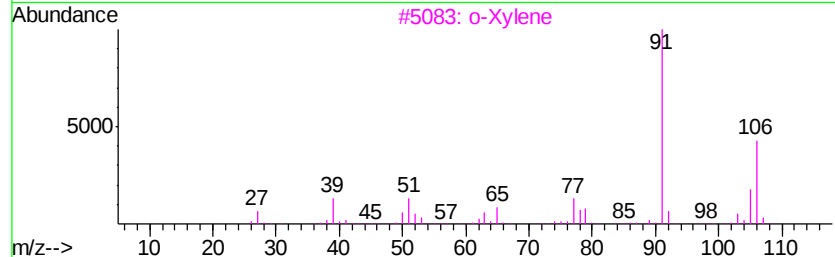
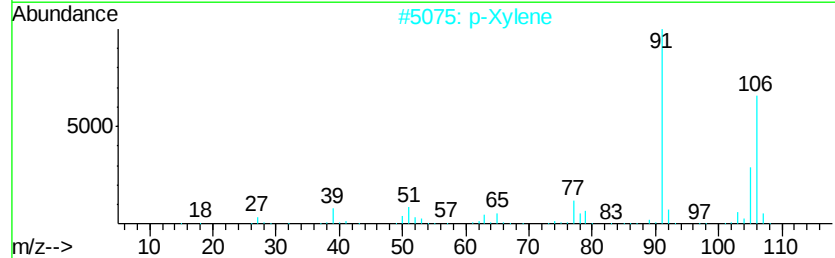
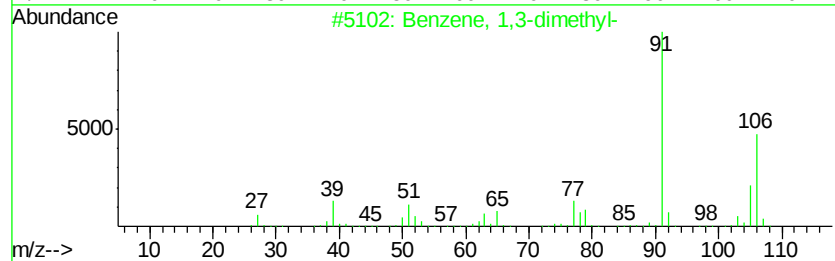
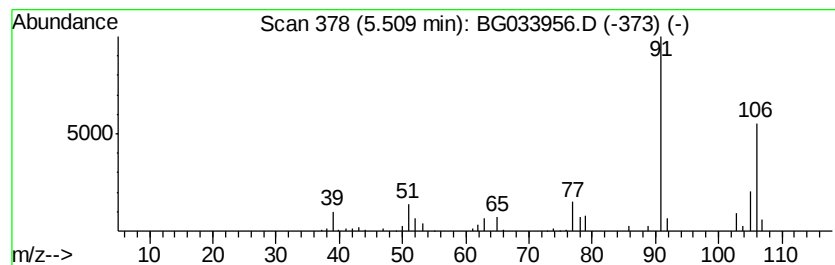
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	6.31 ng	150073	1,4-Dichlorobenzene-d4	7.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	95
2		p-Xylene	106	C8H10	000106-42-3	91
3		o-Xylene	106	C8H10	000095-47-6	91
4		Cyclopentene, 1-ethenyl-3-methyl...	106	C8H10	061142-07-2	86
5		1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	83



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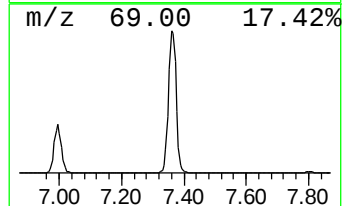
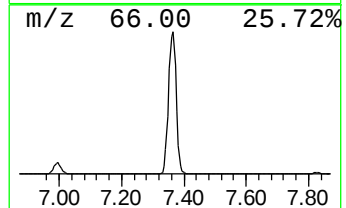
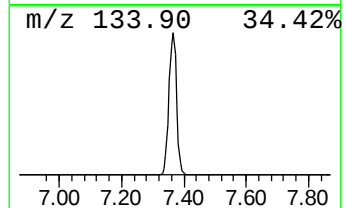
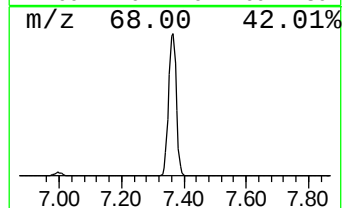
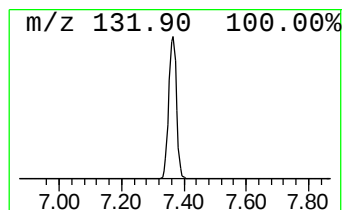
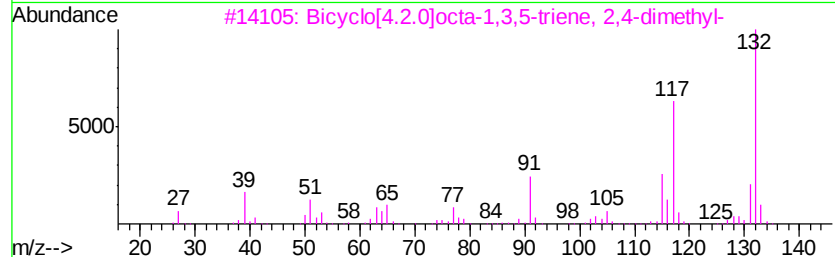
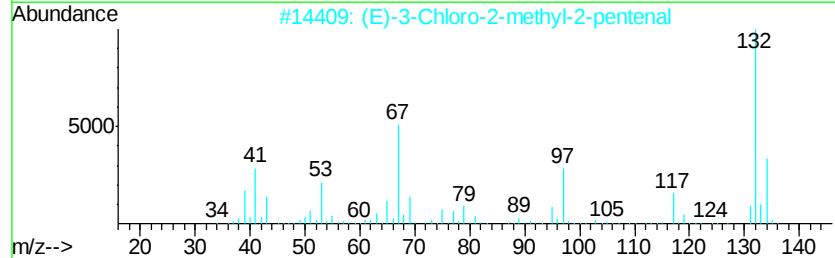
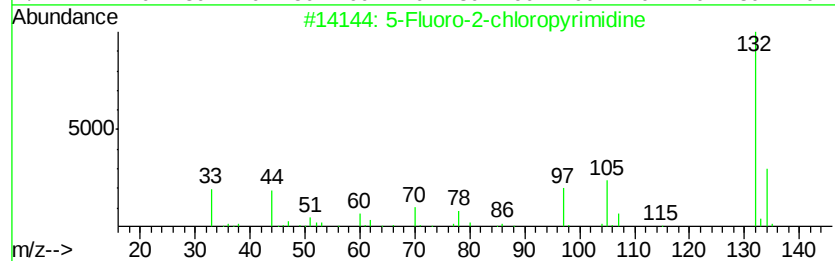
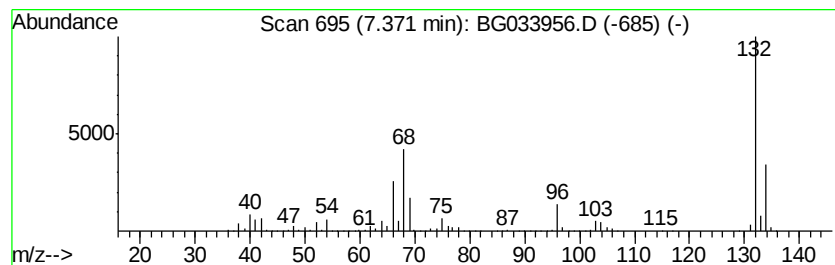
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	91.18 ng	2167670	1,4-Dichlorobenzene-d4	7.82

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	9
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		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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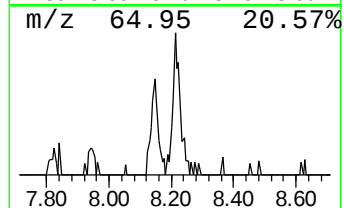
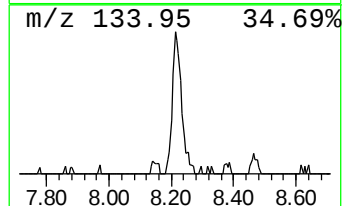
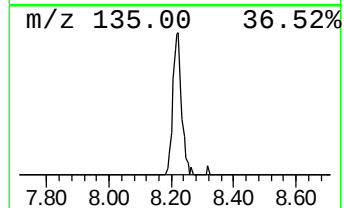
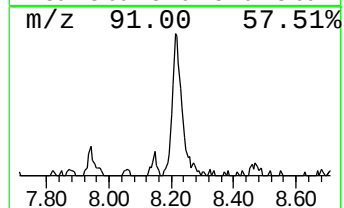
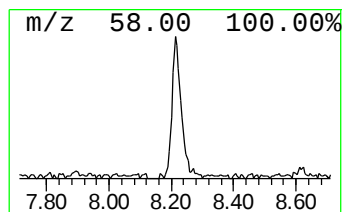
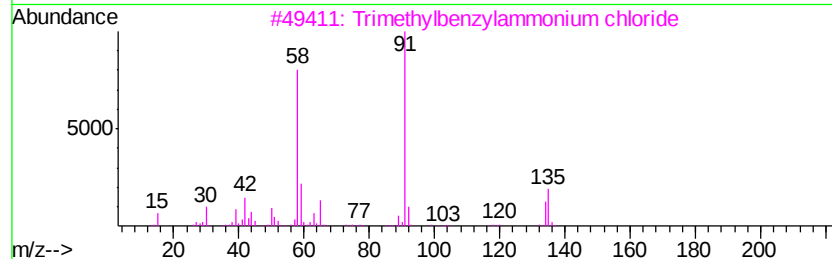
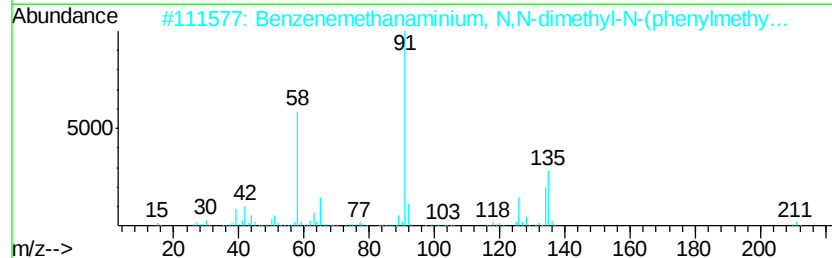
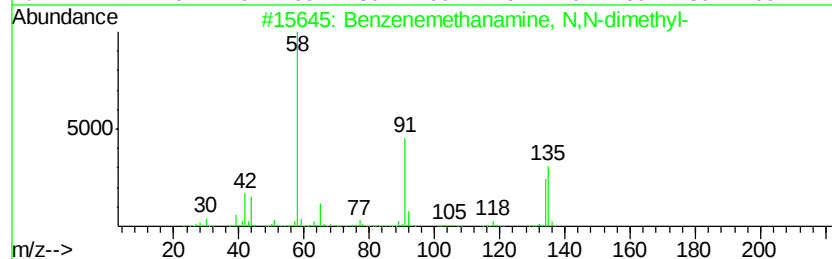
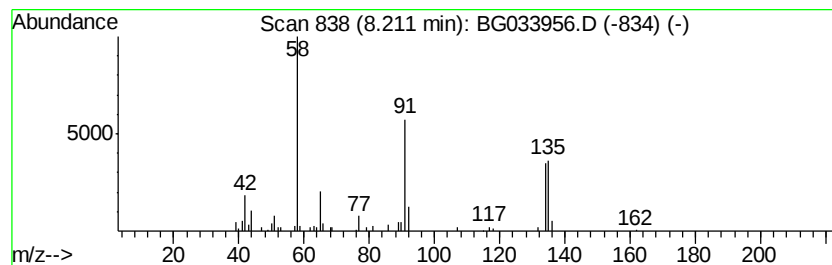
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzenemethanamine, N,N-dim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.21	3.74 ng	88834	1,4-Dichlorobenzene-d4	7.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenemethanamine, N,N-dimethyl-	135	C9H13N	000103-83-3	87
2		Benzenemethanaminium, N,N-dimeth...	261	C16H20ClN	000100-94-7	50
3		Trimethylbenzylammonium chloride	185	C10H16ClN	000056-93-9	43
4		Benzene, butyl-	134	C10H14	000104-51-8	14
5		Benzene, (2-methoxyethenyl)-, (Z)-	134	C9H10O	014371-19-8	14



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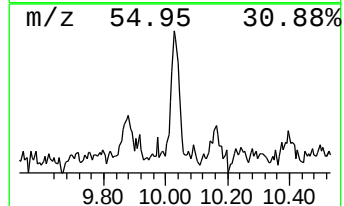
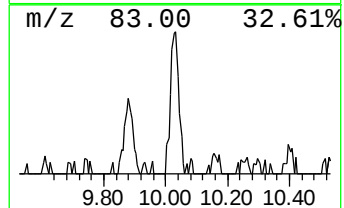
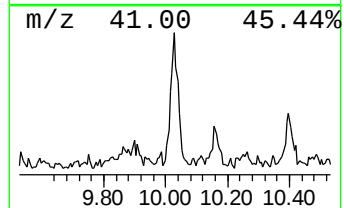
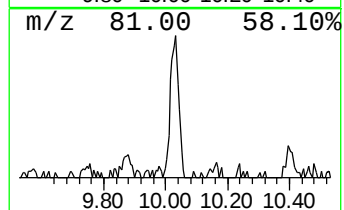
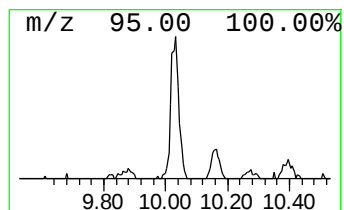
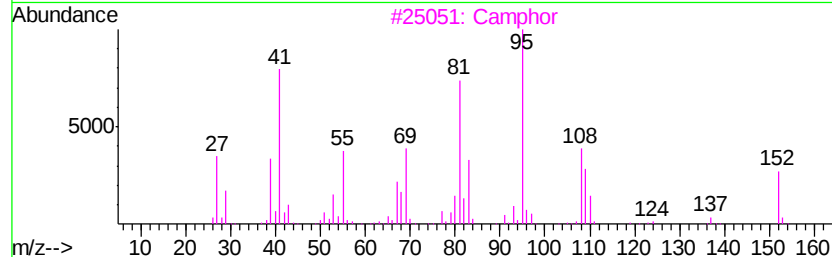
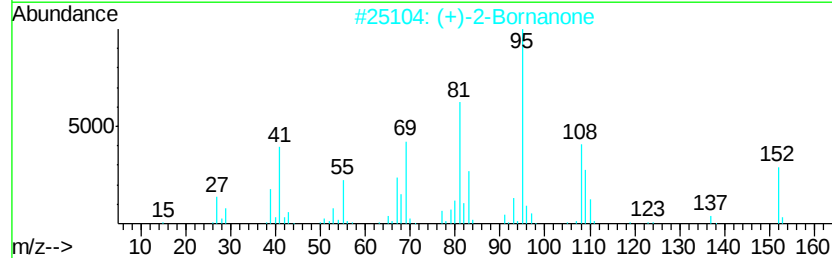
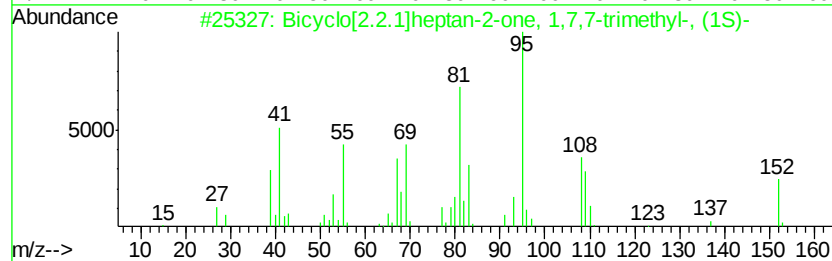
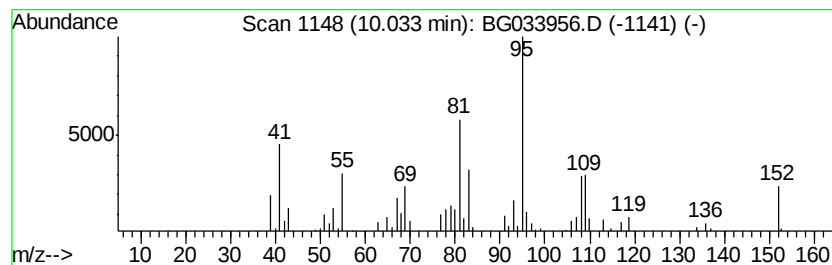
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Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	3.01 ng	95775	Naphthalene-d8	10.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	91
2		(+)-2-Bornanone	152	C10H16O	000464-49-3	87
3		Camphor	152	C10H16O	000076-22-2	83
4		5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	50
5		Tricyclo[2.2.1.0(2,6)]heptan-3-o...	152	C10H16O	062560-53-6	49



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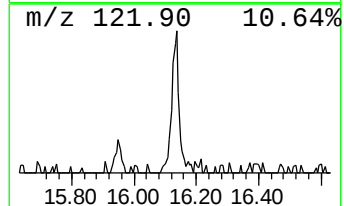
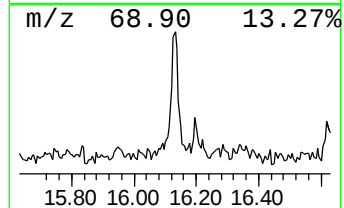
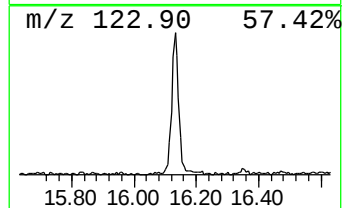
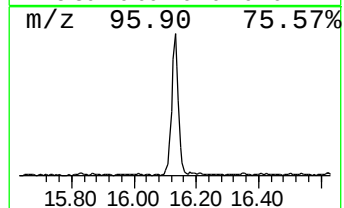
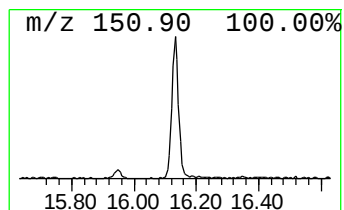
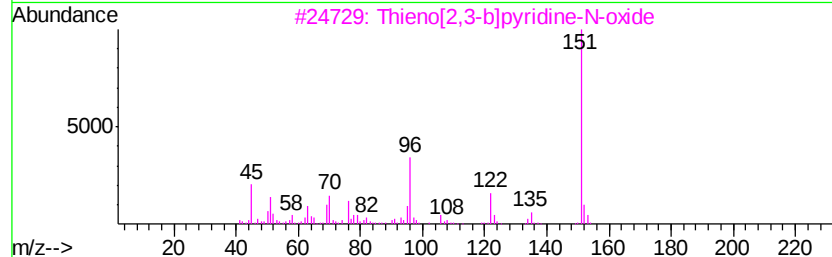
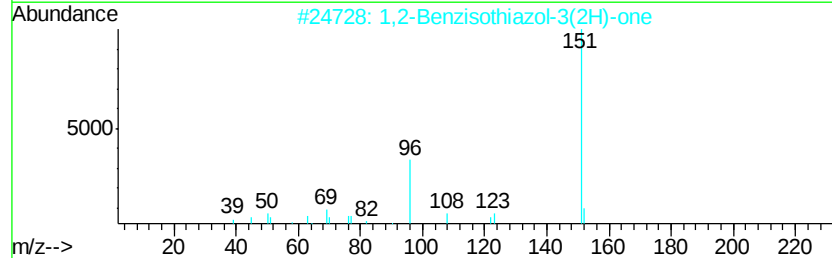
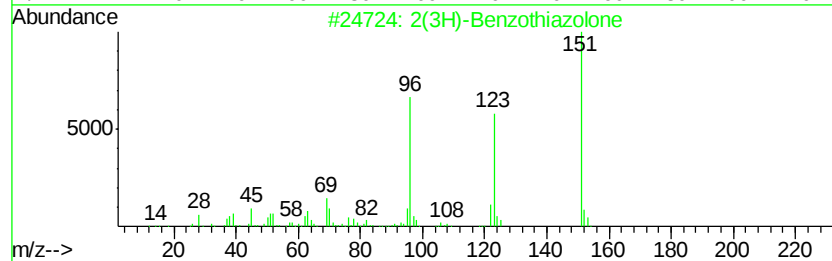
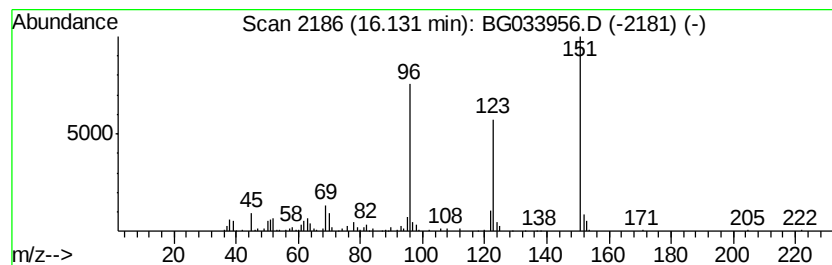
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2(3H)-Benzothiazolone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	3.31 ng	187741	Phenanthrene-d10	17.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	96
2		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
3		Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	42
4		4-Mercaptoimidazo[4,5-c]pyridine	151	C6H5N3S	034550-51-1	27
5		1H-Imidazo[4,5-b]pyridine-2-thiol	151	C6H5N3S	029448-81-5	27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033956.D
Acq On : 24 Apr 2018 16:15
Operator : SJ/JU
Sample : J2471-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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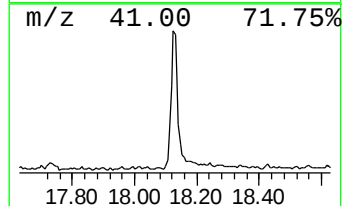
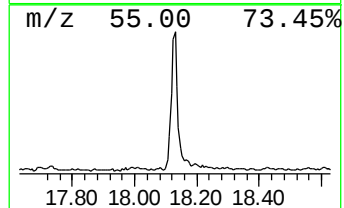
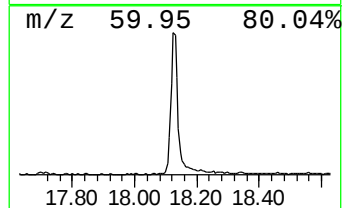
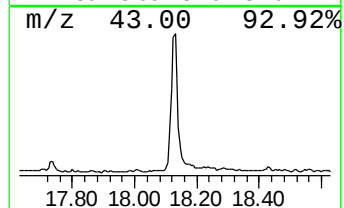
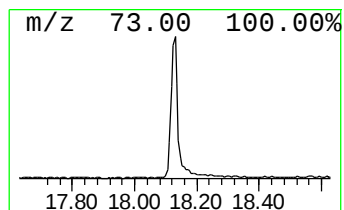
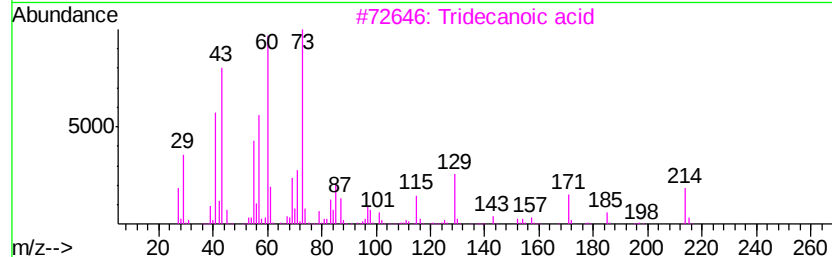
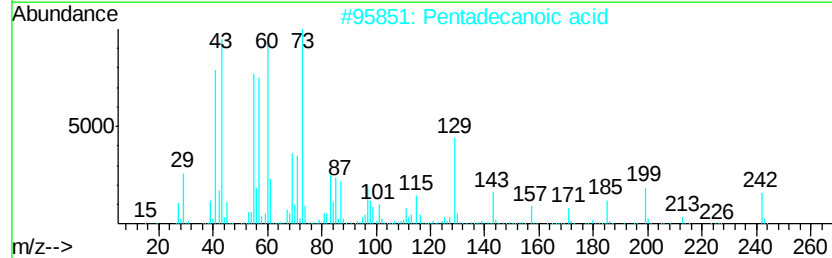
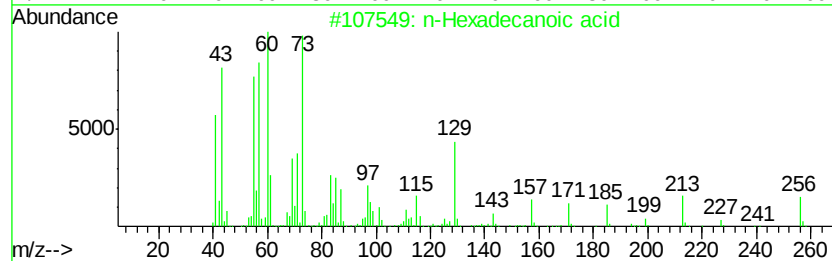
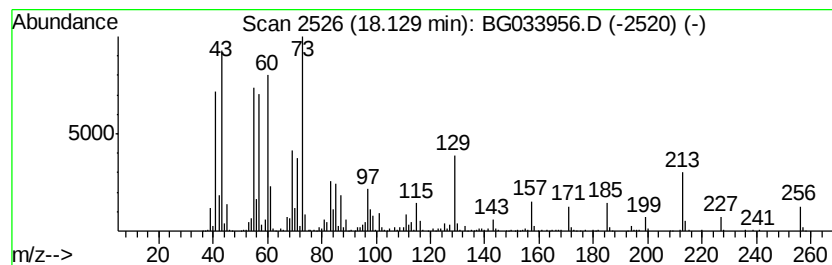
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	16.41 ng	930999	Phenanthrene-d10	17.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033956.D
Acq On : 24 Apr 2018 16:15
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Sample : J2471-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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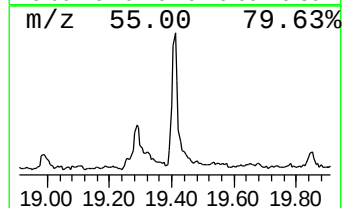
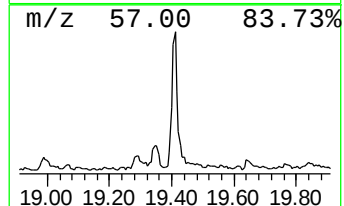
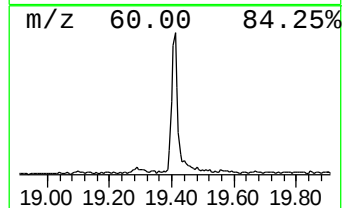
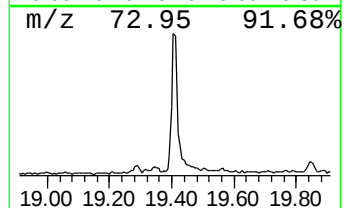
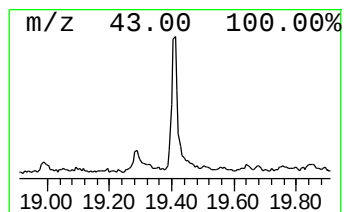
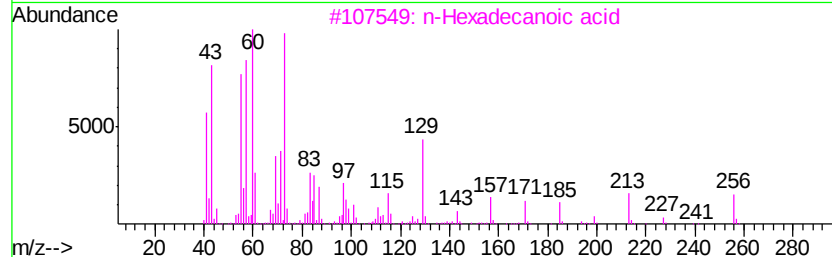
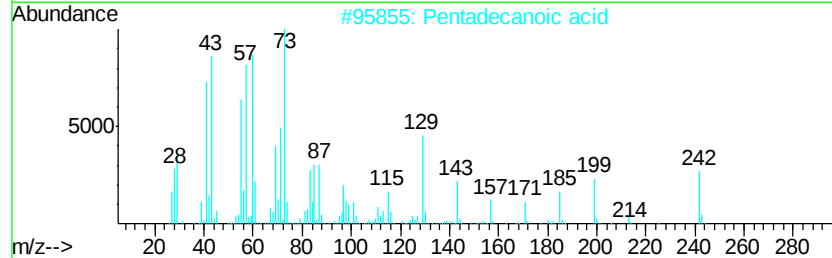
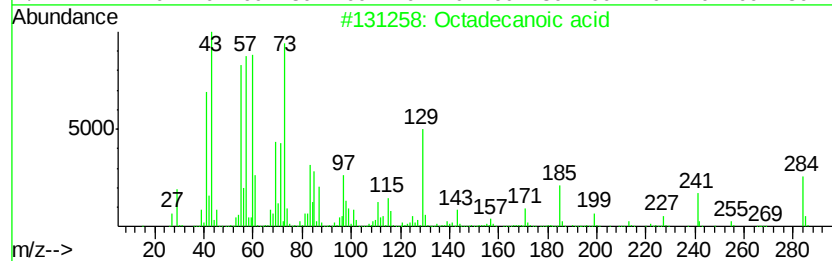
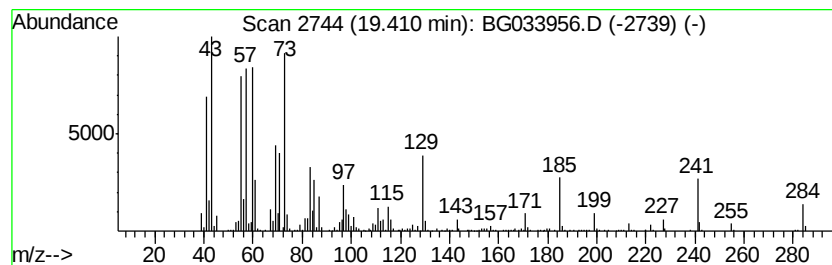
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.41	7.84 ng	575337	Chrysene-d12	21.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033956.D
Acq On : 24 Apr 2018 16:15
Operator : SJ/JU
Sample : J2471-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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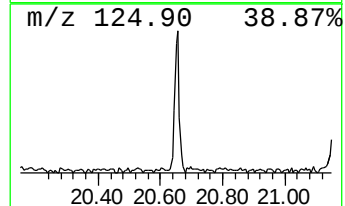
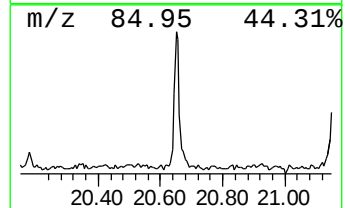
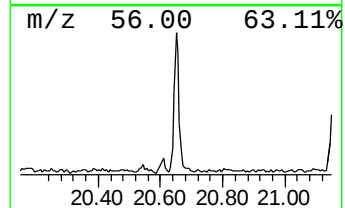
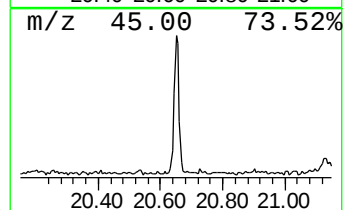
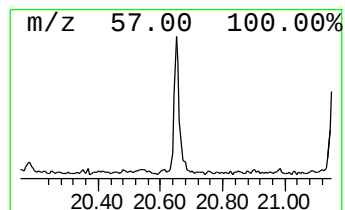
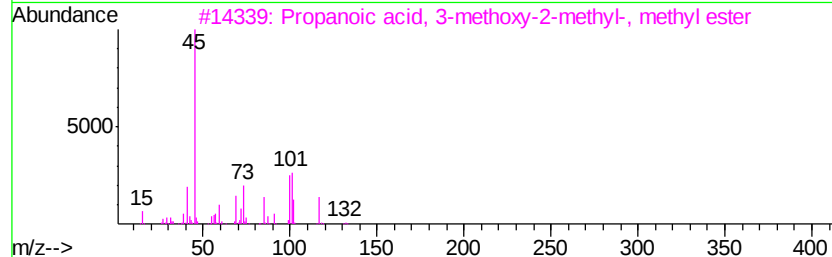
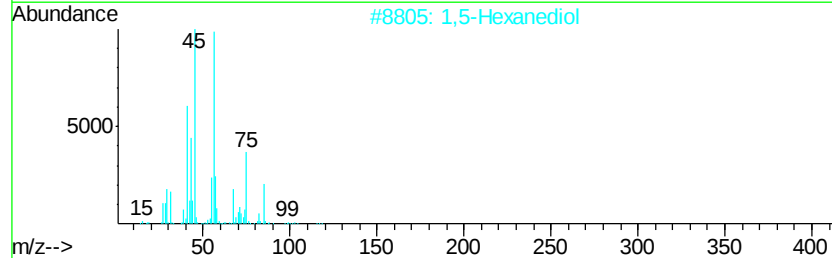
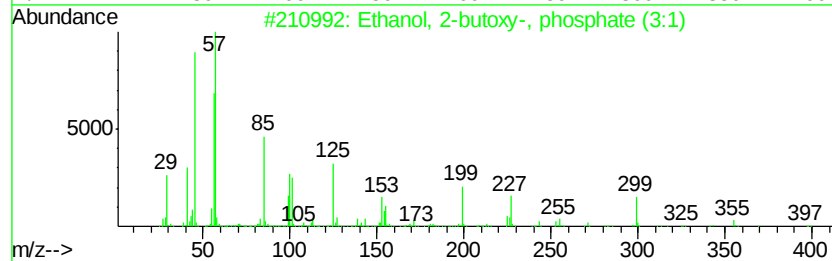
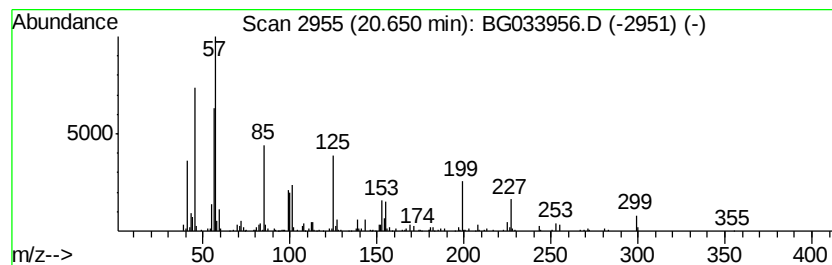
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Ethanol, 2-butoxy-, phospho... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.65	3.01 ng	221086	Chrysene-d12	21.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	83
2		1,5-Hexanediol	118	C6H14O2	000928-40-5	35
3		Propanoic acid, 3-methoxy-2-meth...	132	C6H12O3	003852-11-7	25
4		Di-sec-butyl ether	130	C8H18O	006863-58-7	22
5		1-Methoxy-5-heptafluorobutyrylox...	328	C11H15F7O3	1000216-63-3	14



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
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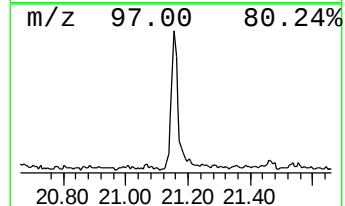
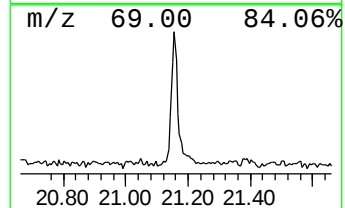
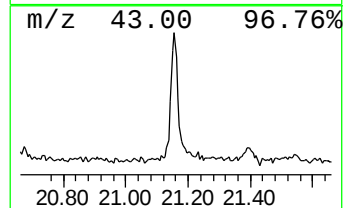
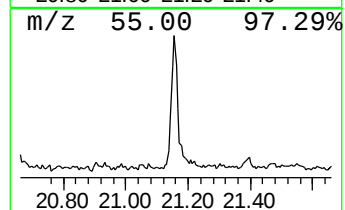
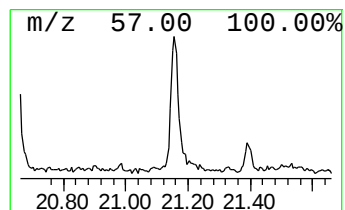
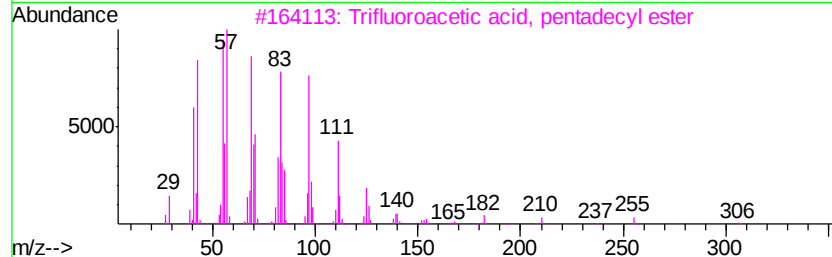
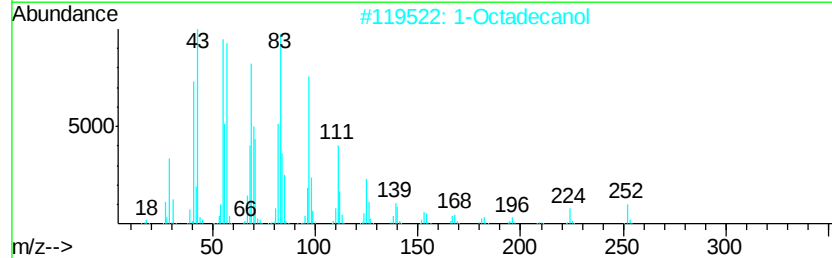
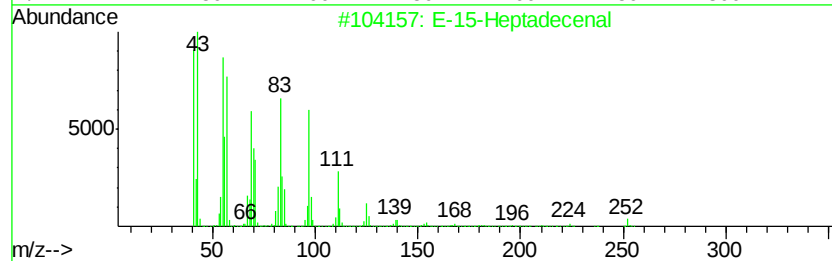
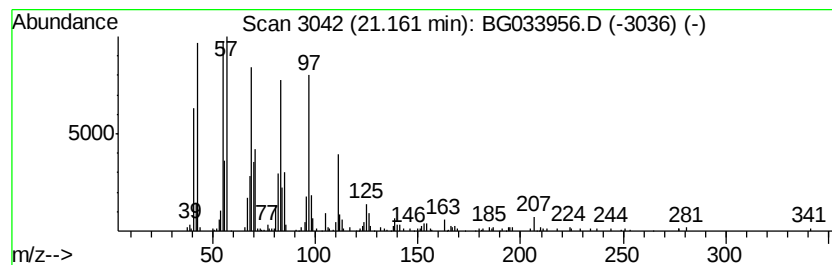
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 E-15-Heptadecenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.16	4.07 ng	298505	Chrysene-d12	21.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	99
2	1-Octadecanol	270	C18H38O	000112-92-5	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	94



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033956.D
Acq On : 24 Apr 2018 16:15
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Misc :
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ClientSampleId :
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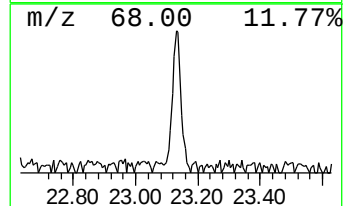
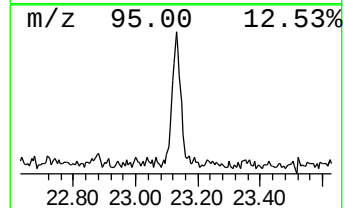
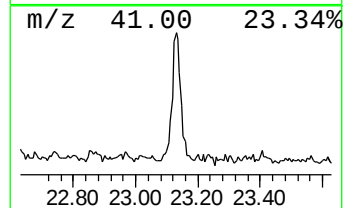
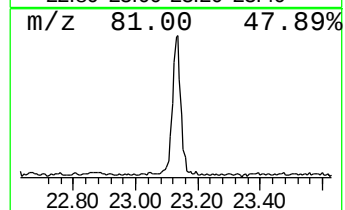
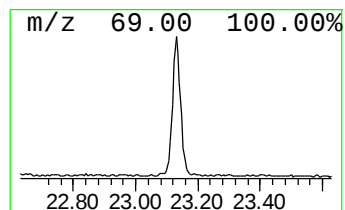
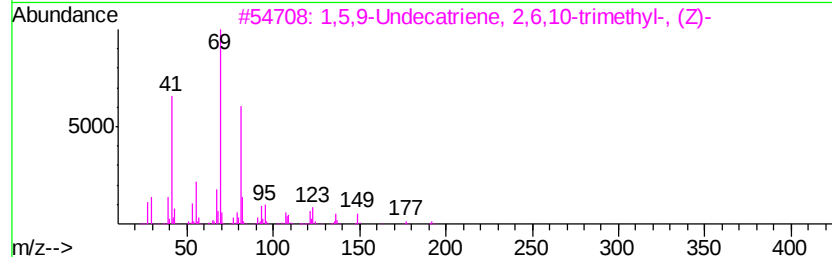
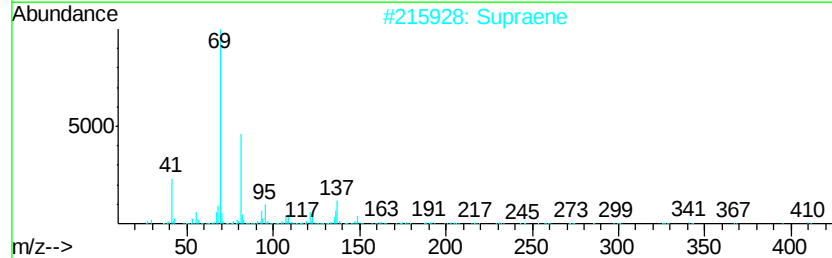
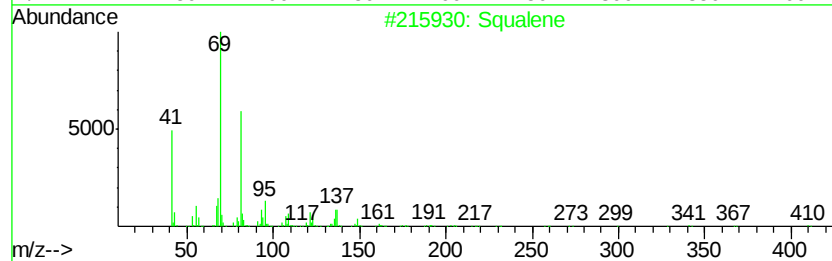
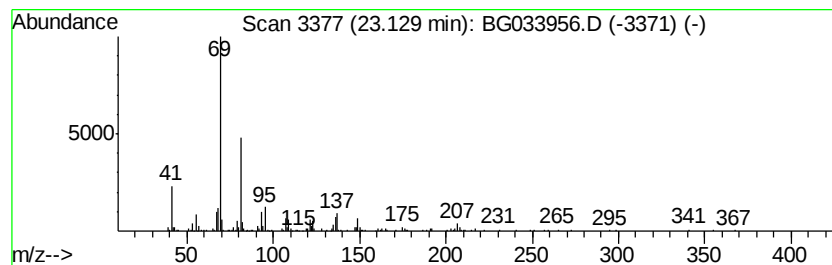
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	3.36 ng	247518	Perylene-d12	24.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		Supraene	410	C30H50	007683-64-9	83
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
4		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
5		5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
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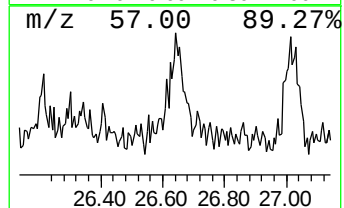
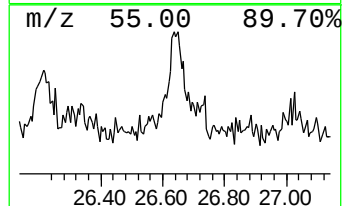
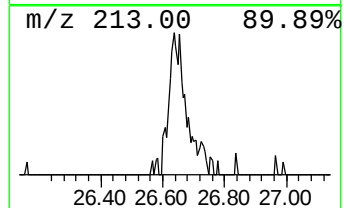
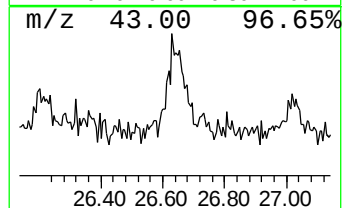
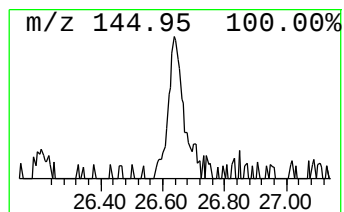
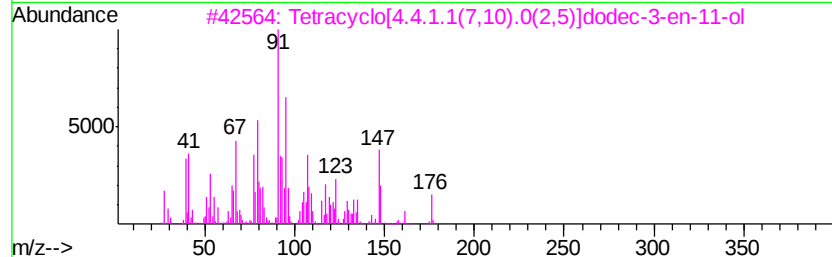
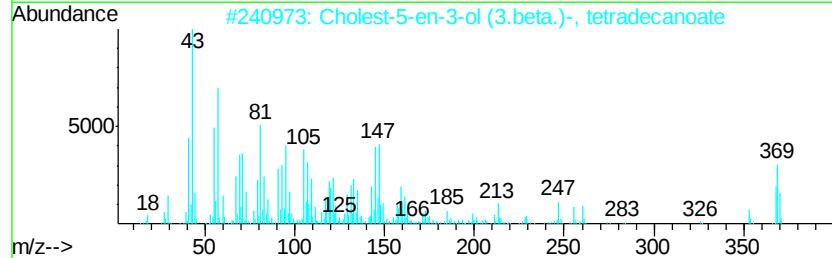
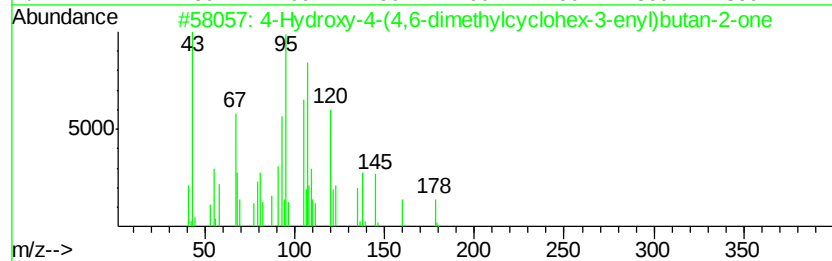
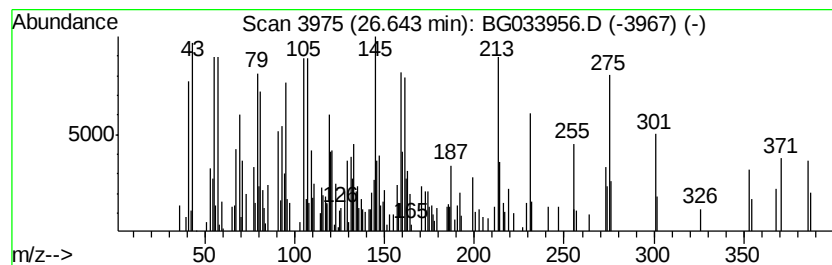
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown26.64 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.64	2.64 ng	194055	Perylene-d12	24.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H20O2	002316-79-2	22
2		Cholest-5-en-3-ol (3.beta.)-, te...	597	C41H72O2	001989-52-2	20
3		Tetracyclo[4.4.1.1(7,10).0(2,5)]...	176	C12H16O	1000184-98-8	15
4		2,4-Hexadienamide, N-(4-methylph...	201	C13H15NO	1000362-68-5	14
5		Cyclopentane-3'-spiropentacyclo[...	376	C28H40	1000150-19-8	14



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG042418\
 Data File : BG033956.D
 Acq On : 24 Apr 2018 16:15
 Operator : SJ/JU
 Sample : J2471-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MH-6

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.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
2-Pentanone, 4-hy...	4.99	3.1	ng	72833	1	7.82	475474	20.0
Benzene, 1,3-dime...	5.51	6.3	ng	150073	1	7.82	475474	20.0
unknown7.37	7.37	91.2	ng	2167670	1	7.82	475474	20.0
Benzenemethanamin...	8.21	3.7	ng	88834	1	7.82	475474	20.0
Bicyclo[2.2.1]hep...	10.03	3.0	ng	95775	2	10.61	636959	20.0
2(3H)-Benzothiazo...	16.13	3.3	ng	187741	4	17.21	1134680	20.0
n-Hexadecanoic acid	18.13	16.4	ng	930999	4	17.21	1134680	20.0
Octadecanoic acid	19.41	7.8	ng	575337	5	21.47	1467600	20.0
Ethanol, 2-butoxy...	20.65	3.0	ng	221086	5	21.47	1467600	20.0
E-15-Heptadecenal	21.16	4.1	ng	298505	5	21.47	1467600	20.0
Squalene	23.13	3.4	ng	247518	6	24.52	1471850	20.0
unknown26.64	26.64	2.6	ng	194055	6	24.52	1471850	20.0