

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
 Data File : BG038656.D
 Acq On : 17 Dec 2018 10:26
 Operator : JU/SJ
 Sample : J6424-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EB12_12-14

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-BG121218.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	3.734	107	110	118	rVB2	14433	23237	1.28%	0.262%
2	5.144	345	350	358	rVB	20904	35239	1.94%	0.398%
3	5.609	422	429	439	rVB	369388	623616	34.26%	7.039%
4	7.213	694	702	716	rVB	386949	725073	39.84%	8.184%
5	7.589	758	766	775	rVB	356473	637417	35.02%	7.195%
6	8.059	839	846	853	rBV	72802	124374	6.83%	1.404%
7	8.382	893	901	911	rBV	274860	492337	27.05%	5.557%
8	9.234	1038	1046	1055	rBV	232526	436592	23.99%	4.928%
9	10.873	1319	1325	1333	rBV	87087	164398	9.03%	1.856%
10	13.317	1733	1741	1756	rBV	607534	991123	54.45%	11.187%
11	14.140	1876	1881	1887	rBV	63759	94946	5.22%	1.072%
12	14.698	1969	1976	1986	rBV2	149751	248323	13.64%	2.803%
13	16.184	2223	2229	2245	rBV	514288	805453	44.25%	9.091%
14	17.442	2437	2443	2453	rBV2	214459	345347	18.97%	3.898%
15	18.305	2584	2590	2600	rBV4	12440	21401	1.18%	0.242%
16	19.710	2825	2829	2835	rBV	70360	80717	4.43%	0.911%
17	20.045	2880	2886	2895	rVB	1418383	1820079	100.00%	20.543%
18	20.750	3002	3006	3010	rVB	50568	57373	3.15%	0.648%
19	20.808	3010	3016	3020	rBV	16115	18776	1.03%	0.212%
20	21.314	3095	3102	3115	rBV2	23004	47937	2.63%	0.541%
21	21.719	3165	3171	3181	rVB2	235940	408242	22.43%	4.608%
22	21.866	3190	3196	3202	rVB	20855	30845	1.69%	0.348%
23	22.477	3294	3300	3307	rBV	21559	36519	2.01%	0.412%
24	23.176	3409	3419	3426	rBV2	26347	56396	3.10%	0.637%
25	23.987	3548	3557	3566	rBV3	23937	58788	3.23%	0.664%
26	24.945	3711	3720	3722	rBV3	19121	33982	1.87%	0.384%
27	25.021	3724	3733	3749	rVB2	133654	396707	21.80%	4.478%
28	26.096	3906	3916	3924	rVB7	14250	44469	2.44%	0.502%

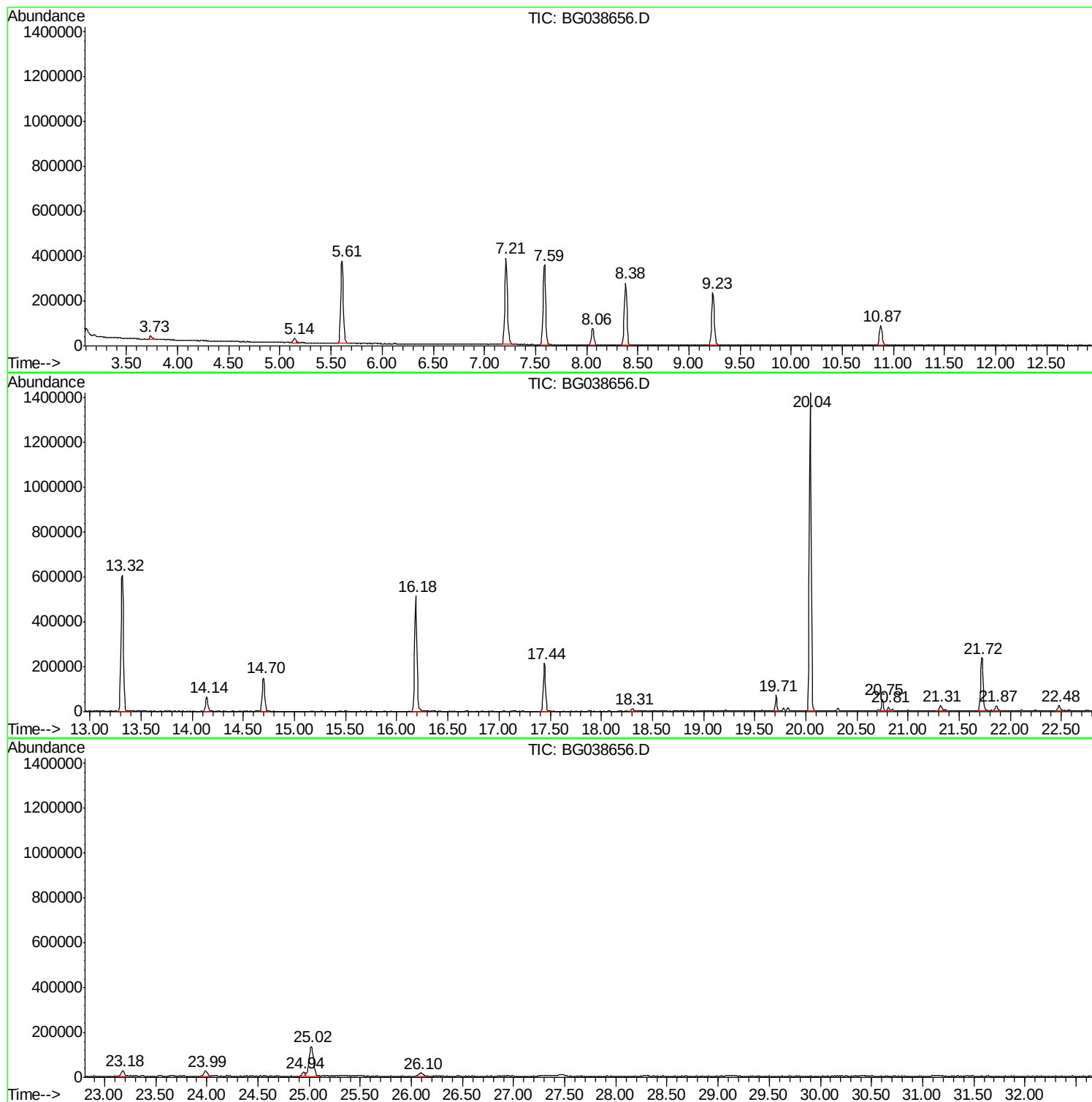
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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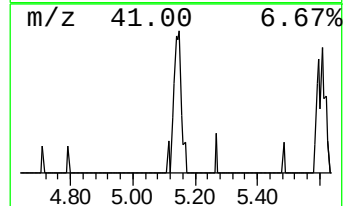
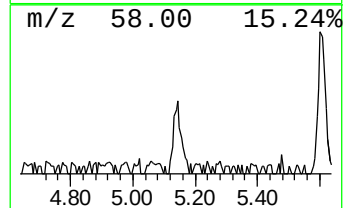
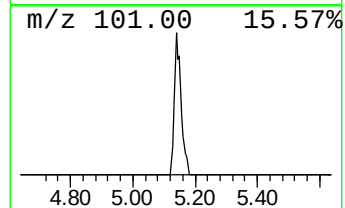
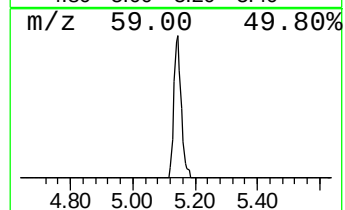
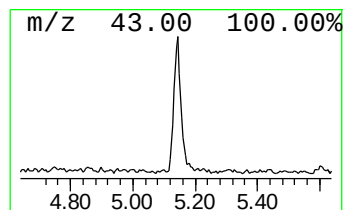
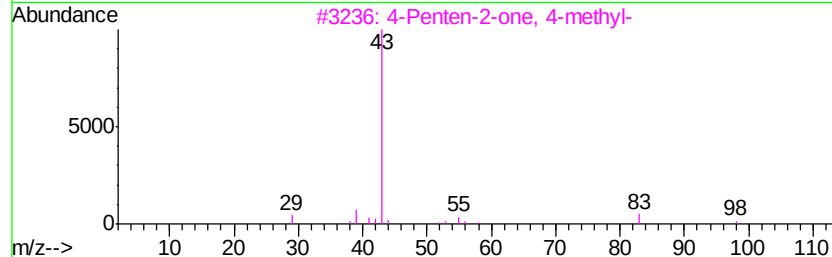
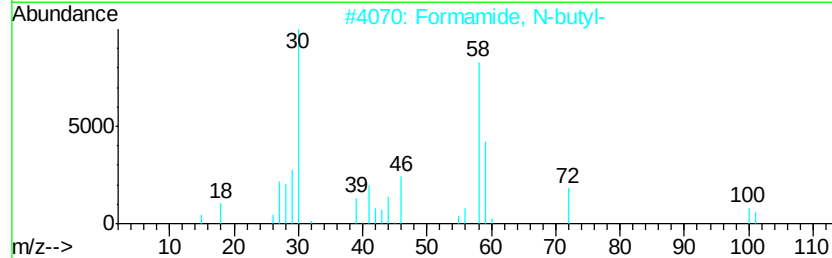
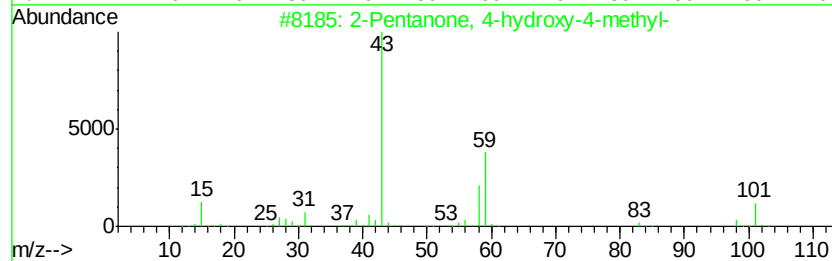
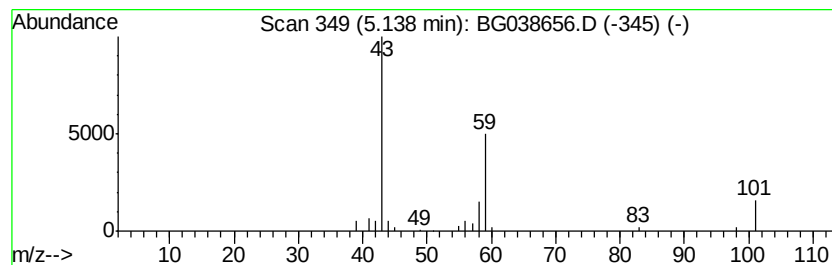
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	5.67 ng	35239	1,4-Dichlorobenzene-d4	8.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
3			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4			Diacetamide	101	C4H7NO2	000625-77-4	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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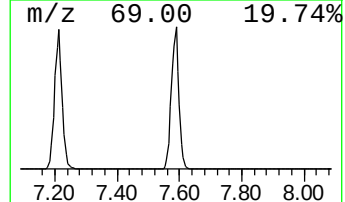
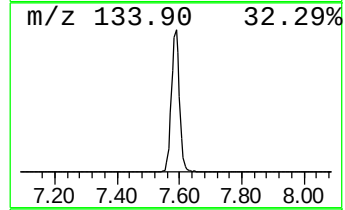
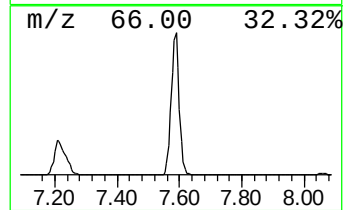
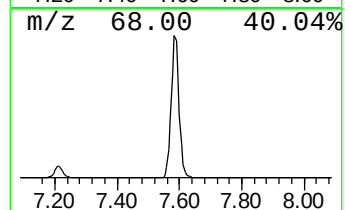
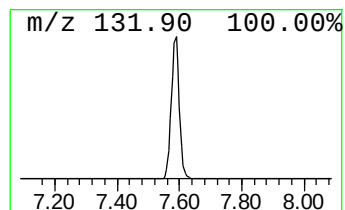
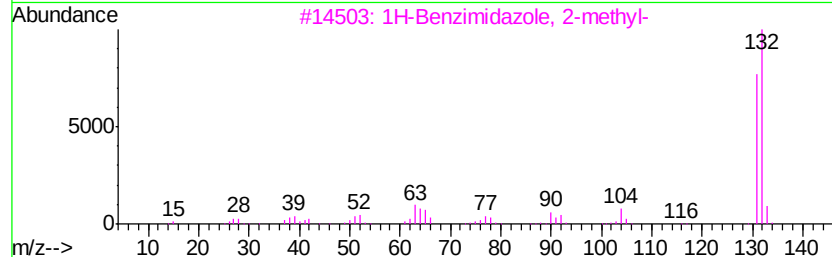
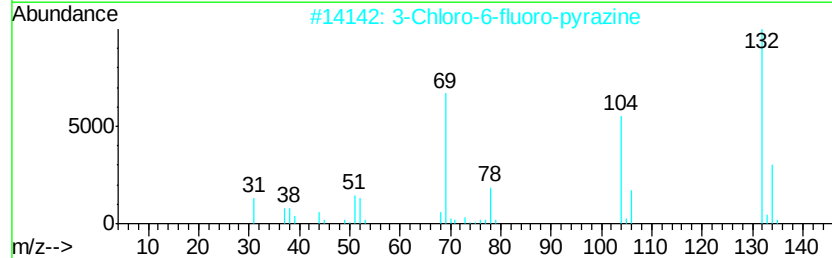
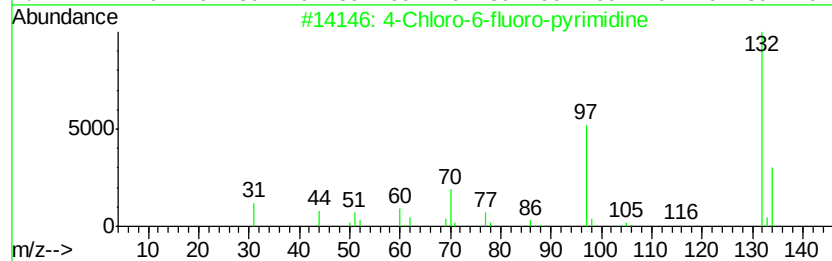
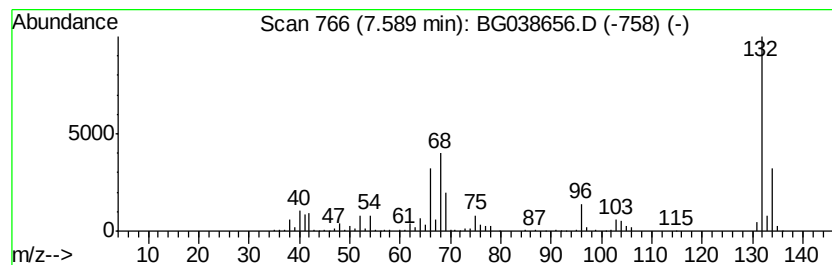
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Peak Number 3 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	102.50 ng	637417	1,4-Dichlorobenzene-d4	8.06

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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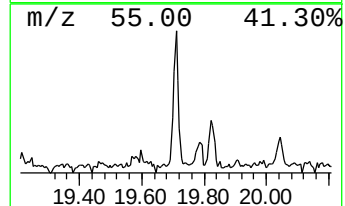
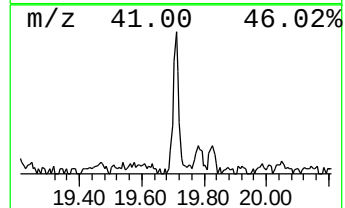
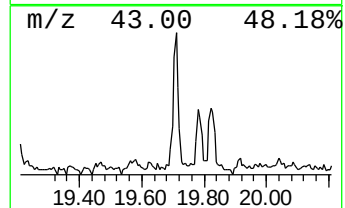
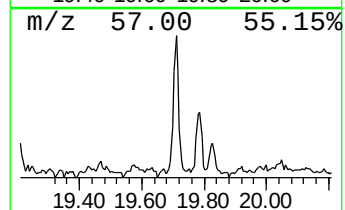
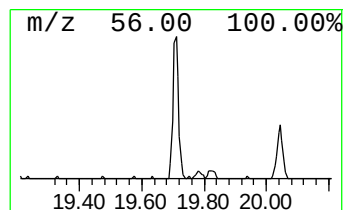
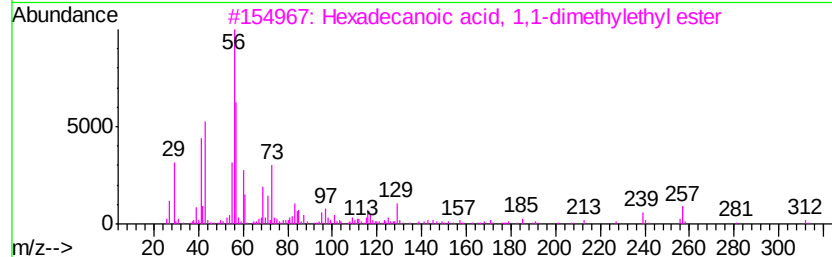
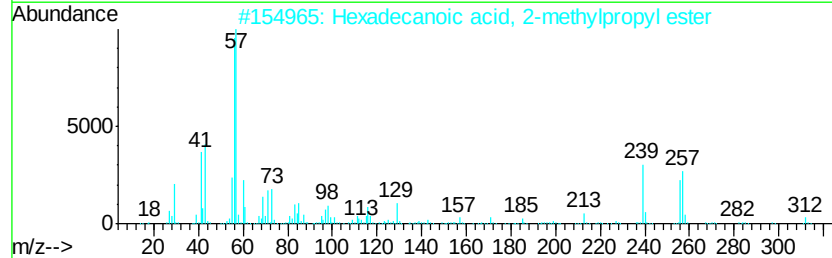
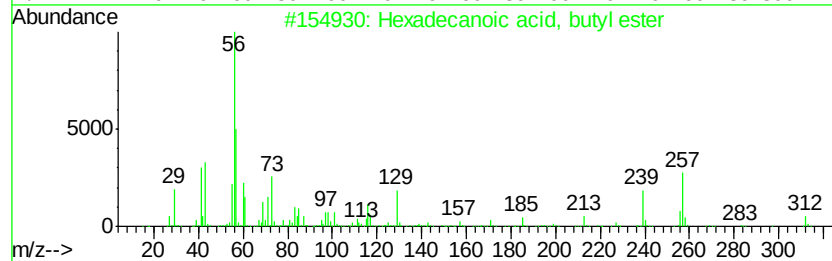
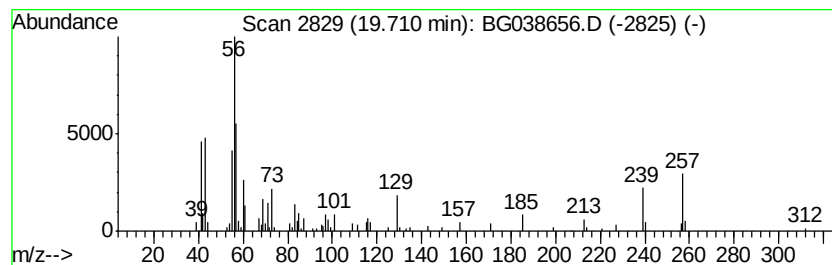
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.71	3.95 ng	80717	Chrysene-d12	21.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	38
4		1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	27
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	27



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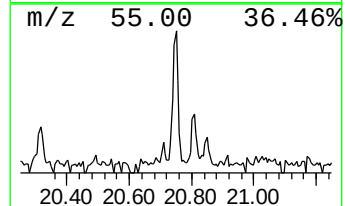
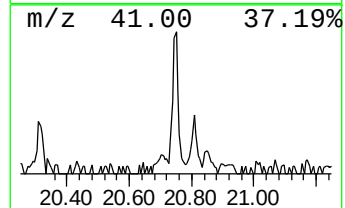
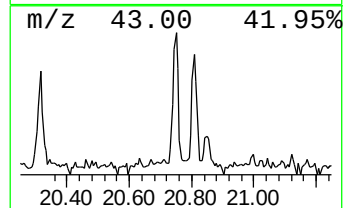
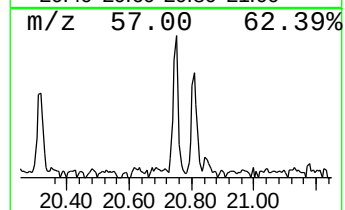
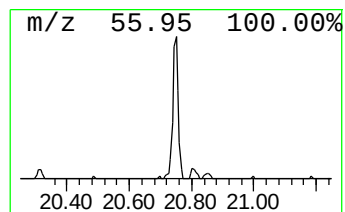
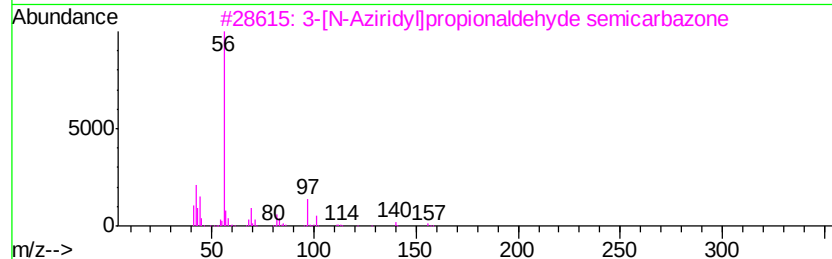
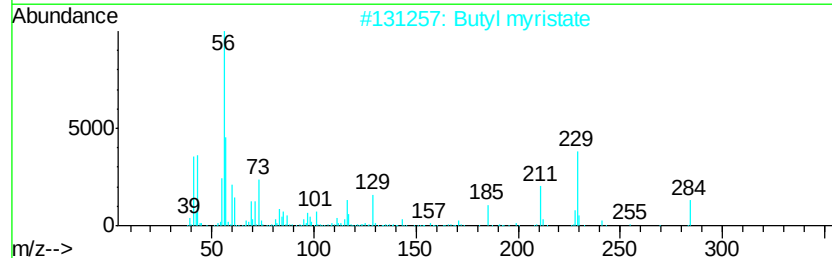
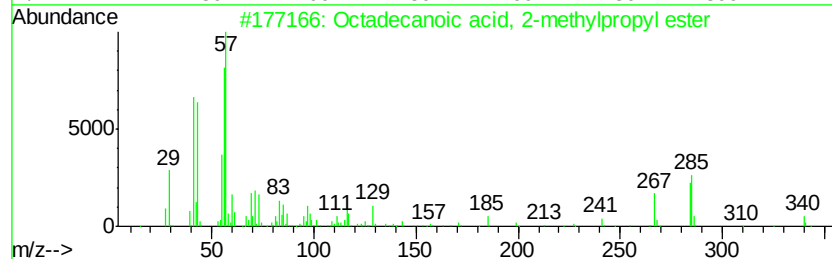
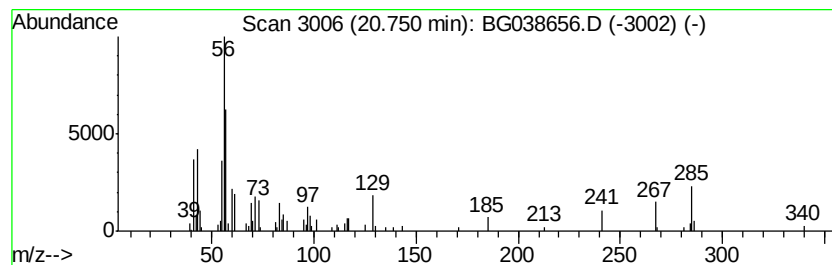
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Peak Number 6 Octadecanoic acid, 2-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.75	2.81 ng	57373	Chrysene-d12	21.72	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	50
2	Butyl myristate	284	C18H36O2	000110-36-1	50
3	3-[N-Aziridyl]propionaldehyde se...	156	C6H12N4O	1000256-01-8	38
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35



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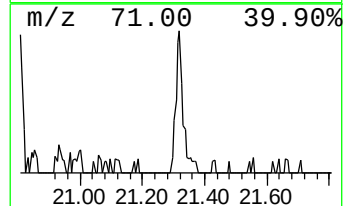
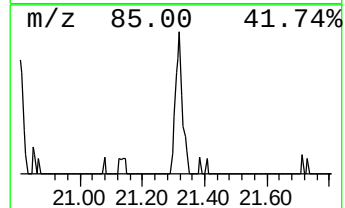
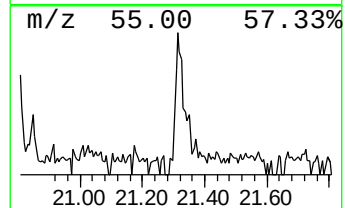
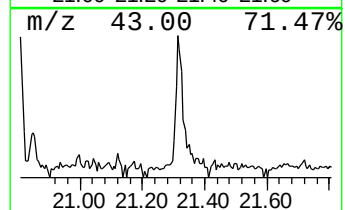
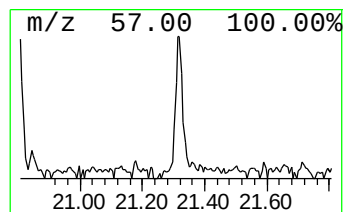
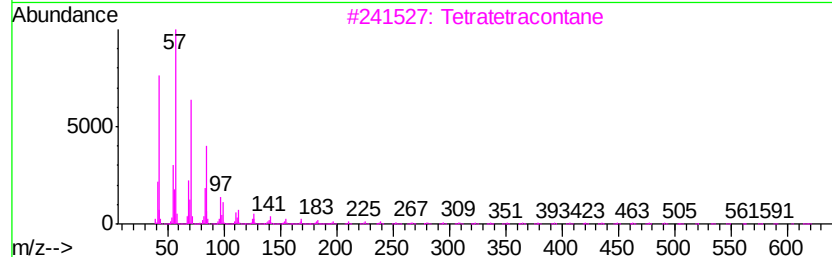
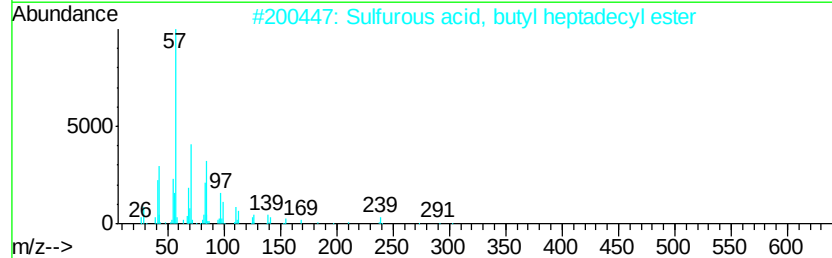
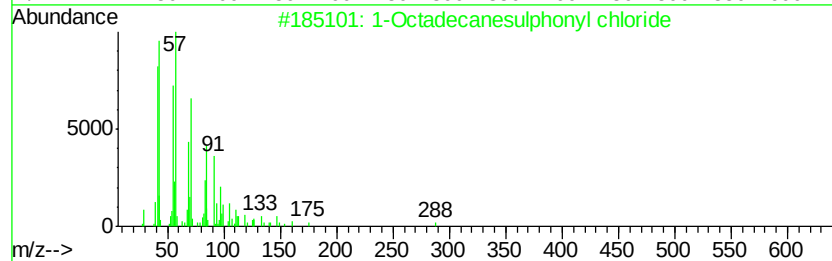
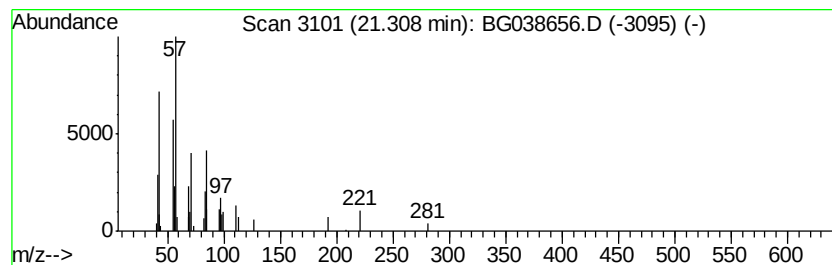
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Peak Number 7 1-Octadecanesulphonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	2.35 ng	47937	Chrysene-d12	21.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	86
2		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	80
3		Tetratetracontane	619	C44H90	007098-22-8	53
4		Hexadecane	226	C16H34	000544-76-3	52
5		Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	52



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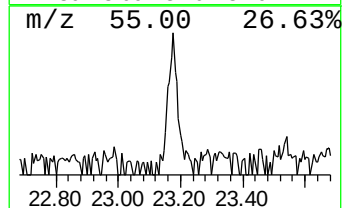
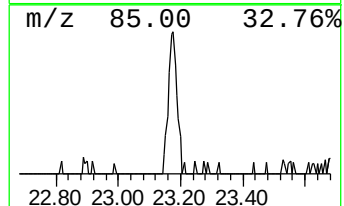
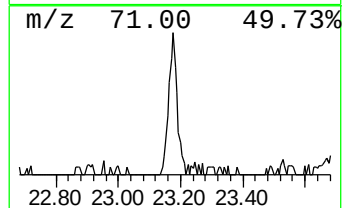
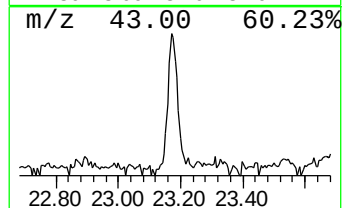
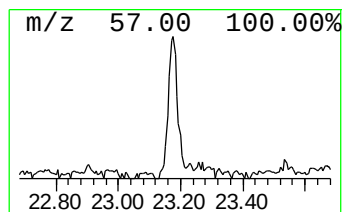
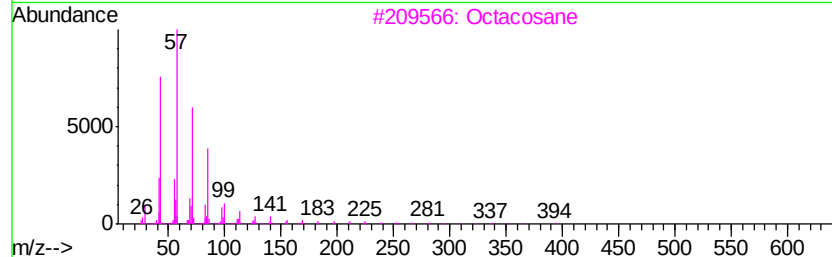
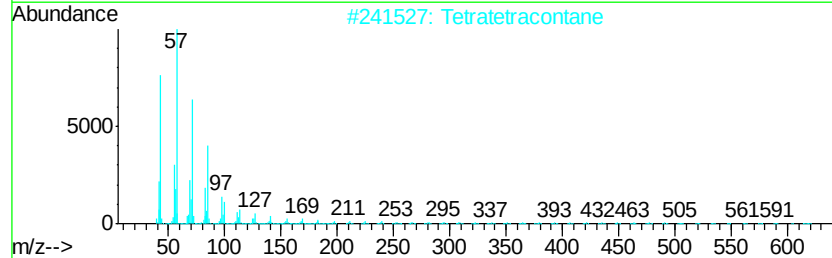
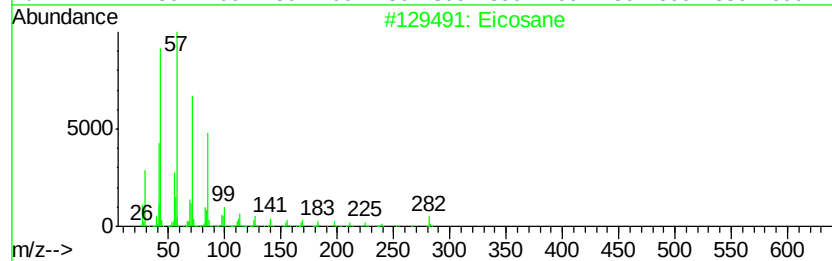
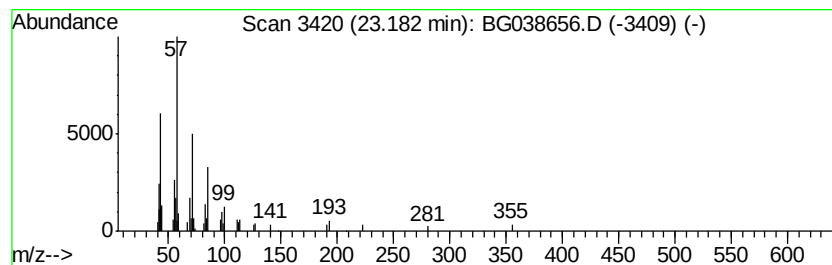
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	2.76 ng	56396	Chrysene-d12	21.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Tetratetracontane	619	C44H90	007098-22-8	83
3		Octacosane	394	C28H58	000630-02-4	83
4		Nonadecane	268	C19H40	000629-92-5	72
5		Hexatriacontane	507	C36H74	000630-06-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038656.D
Acq On : 17 Dec 2018 10:26
Operator : JU/SJ
Sample : J6424-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB12_12-14

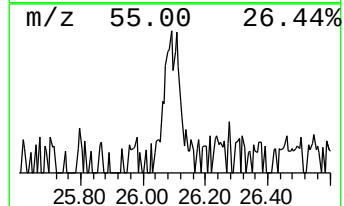
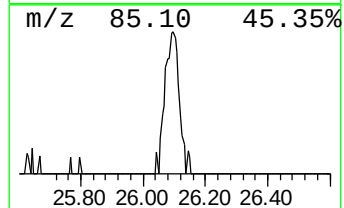
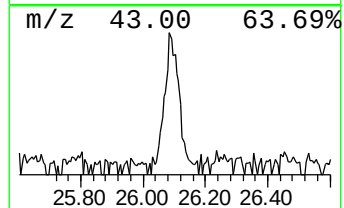
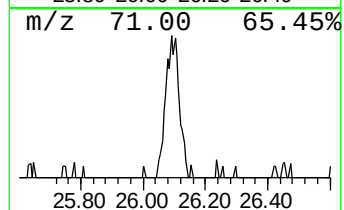
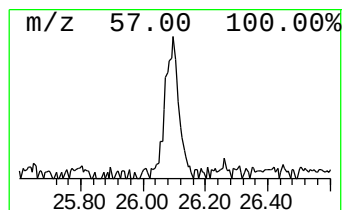
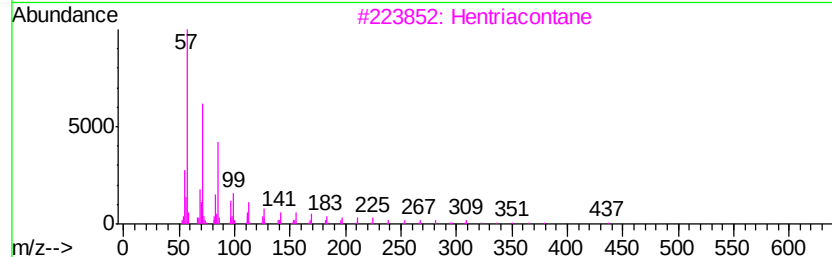
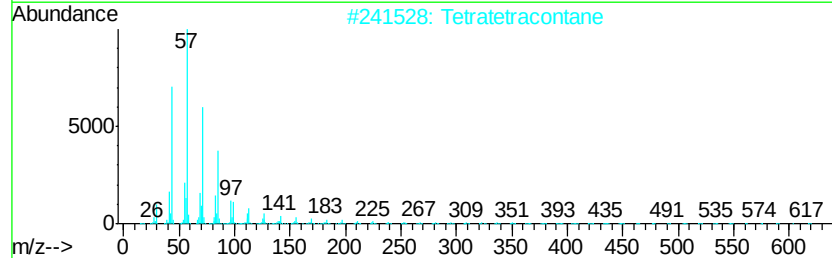
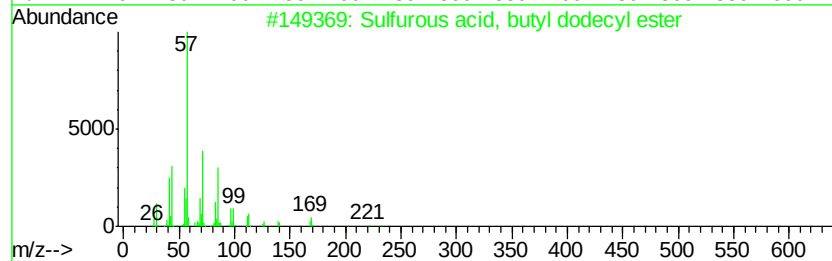
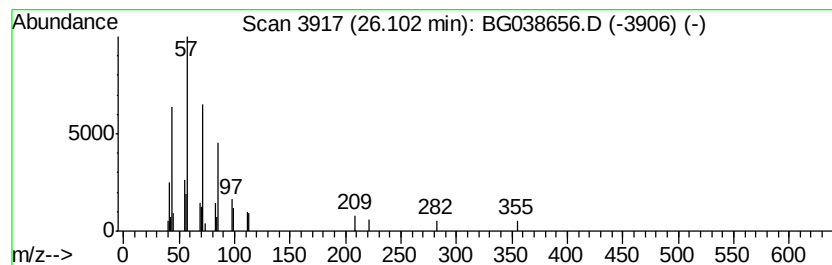
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, butyl dodec... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.10	2.24 ng	44469	Perylene-d12	25.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
2		Tetratetracontane	619	C44H90	007098-22-8	80
3		Hentriacontane	437	C31H64	000630-04-6	80
4		Octacosane	394	C28H58	000630-02-4	72
5		10-Methylnonadecane	282	C20H42	056862-62-5	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038656.D
Acq On : 17 Dec 2018 10:26
Operator : JU/SJ
Sample : J6424-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EB12_12-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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...	5.14	5.7	ng	35239	1	8.06	124374	20.0
unknown7.59	7.59	102.5	ng	637417	1	8.06	124374	20.0
Hexadecanoic acid...	19.71	4.0	ng	80717	5	21.72	408242	20.0
Octadecanoic acid...	20.75	2.8	ng	57373	5	21.72	408242	20.0
1-Octadecanesulph...	21.31	2.4	ng	47937	5	21.72	408242	20.0
Eicosane	23.18	2.8	ng	56396	5	21.72	408242	20.0
Sulfurous acid, b...	26.10	2.2	ng	44469	6	25.02	396707	20.0