

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
 Data File : BG038669.D
 Acq On : 17 Dec 2018 19:02
 Operator : JU/SJ
 Sample : J6391-12
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P001-SS017-0006-01

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	5.139	345	349	357	rBV	21407	38395	3.99%	0.451%
2	5.609	422	429	440	rVB	394448	659708	68.49%	7.751%
3	7.213	694	702	712	rBV	410648	764680	79.38%	8.984%
4	7.589	758	766	777	rBV	377035	684849	71.10%	8.046%
5	8.059	839	846	853	rBV	85599	145091	15.06%	1.705%
6	8.382	893	901	910	rVB	247367	440437	45.72%	5.174%
7	9.234	1038	1046	1059	rBV	246607	459885	47.74%	5.403%
8	10.879	1317	1326	1336	rBV	102389	197817	20.54%	2.324%
9	13.317	1734	1741	1751	rVB	367057	603716	62.67%	7.093%
10	14.140	1876	1881	1887	rBV2	22107	33193	3.45%	0.390%
11	14.698	1969	1976	1986	rVB2	167339	287495	29.85%	3.378%
12	16.185	2223	2229	2243	rBV	426611	668307	69.38%	7.852%
13	17.442	2436	2443	2454	rBV	247697	389774	40.46%	4.579%
14	18.300	2584	2589	2599	rBV3	25189	42796	4.44%	0.503%
15	19.152	2729	2734	2741	rBV5	9835	18774	1.95%	0.221%
16	19.569	2801	2805	2810	rBV4	7645	10819	1.12%	0.127%
17	20.045	2880	2886	2892	rBV	730144	963258	100.00%	11.317%
18	20.315	2923	2932	2936	rBV3	17674	30570	3.17%	0.359%
19	20.809	3010	3016	3021	rBV5	6439	10187	1.06%	0.120%
20	21.320	3096	3103	3112	rBV	78272	145091	15.06%	1.705%
21	21.719	3163	3171	3178	rBV	257127	457401	47.48%	5.374%
22	21.866	3191	3196	3201	rBV3	12976	17216	1.79%	0.202%
23	22.119	3236	3239	3247	rBV8	7069	13100	1.36%	0.154%
24	22.477	3293	3300	3304	rBV	66851	120054	12.46%	1.410%
25	22.518	3304	3307	3320	rVB7	27912	68225	7.08%	0.802%
26	23.176	3413	3419	3424	rVB2	24061	45737	4.75%	0.537%
27	23.376	3445	3453	3458	rVB10	5395	11113	1.15%	0.131%
28	23.547	3475	3482	3488	rBV3	21775	45694	4.74%	0.537%
29	23.987	3547	3557	3567	rBV	90569	210820	21.89%	2.477%
30	24.081	3567	3573	3578	rBV7	13422	32723	3.40%	0.384%
31	24.211	3589	3595	3603	rVB9	7330	18054	1.87%	0.212%
32	24.951	3713	3721	3722	rBV4	18413	33255	3.45%	0.391%
33	25.021	3725	3733	3744	rVB2	145508	416414	43.23%	4.892%
34	25.497	3804	3814	3825	rBV3	34318	106178	11.02%	1.247%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	26.097	3905	3916	3928	rVB5	43879	140685	14.61%	1.653%
36	26.261	3937	3944	3950	rBV9	7895	28117	2.92%	0.330%
37	26.437	3968	3974	3985	rVB7	8908	25159	2.61%	0.296%
38	27.465	4141	4149	4151	rBV7	5990	10718	1.11%	0.126%
39	28.300	4278	4291	4304	rBV8	23520	97425	10.11%	1.145%
40	29.651	4512	4521	4523	rBV6	8485	18811	1.95%	0.221%

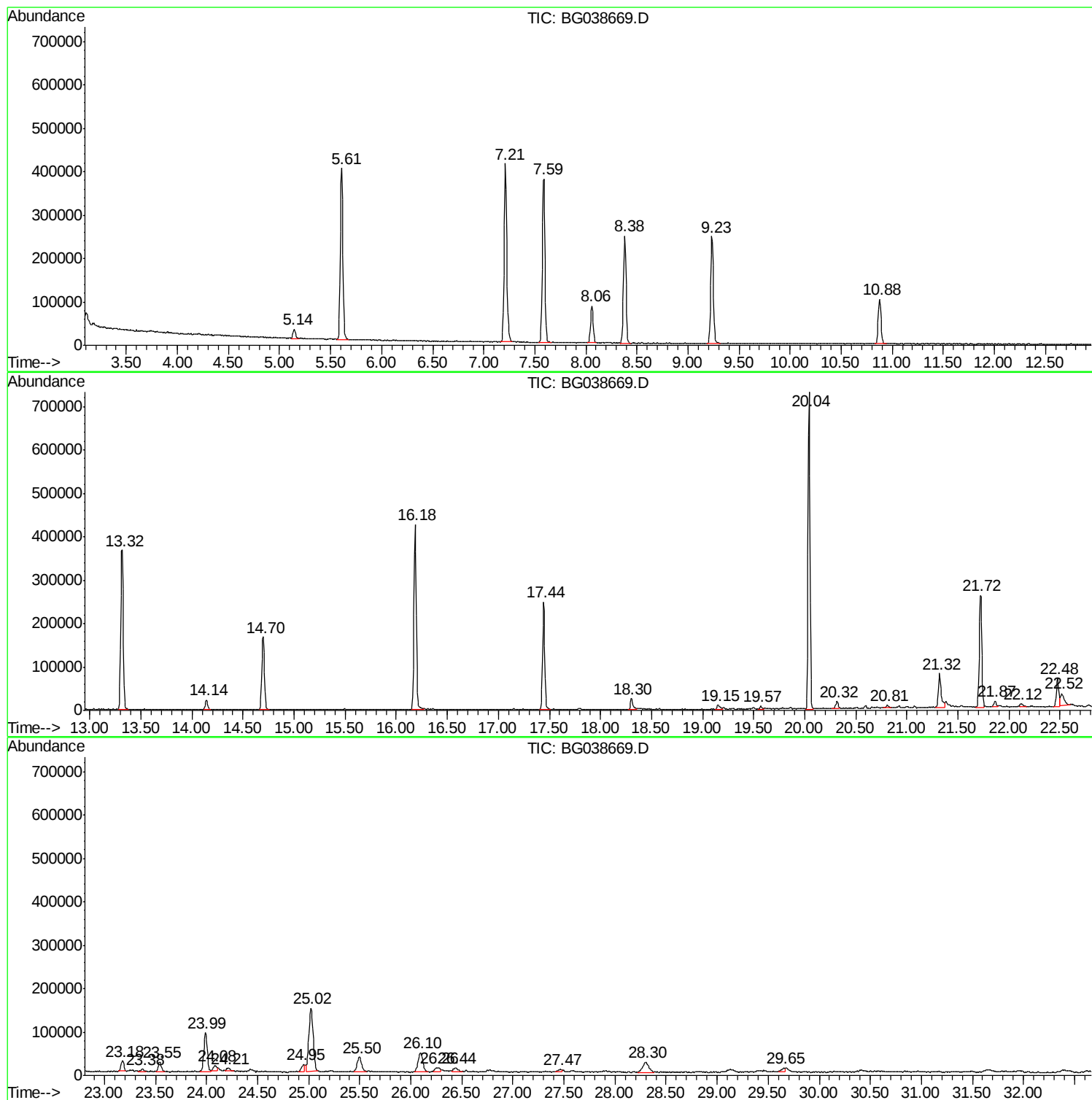
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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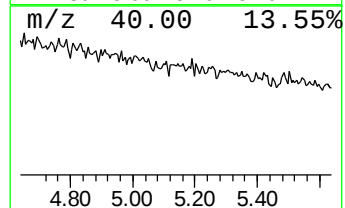
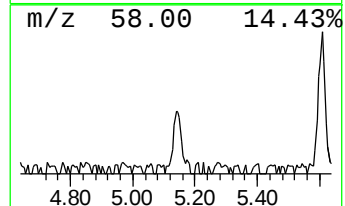
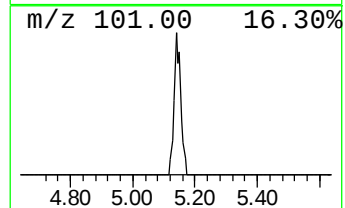
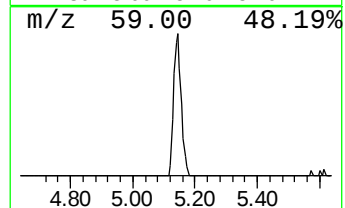
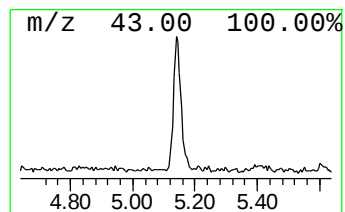
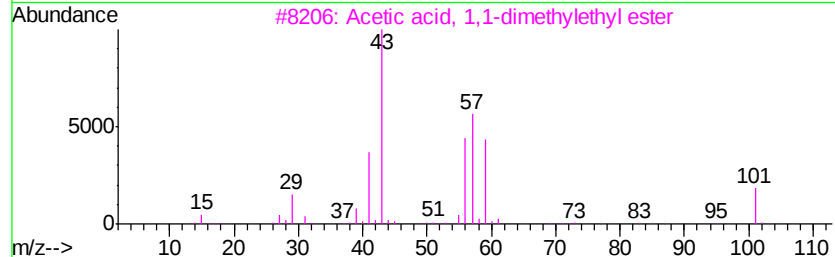
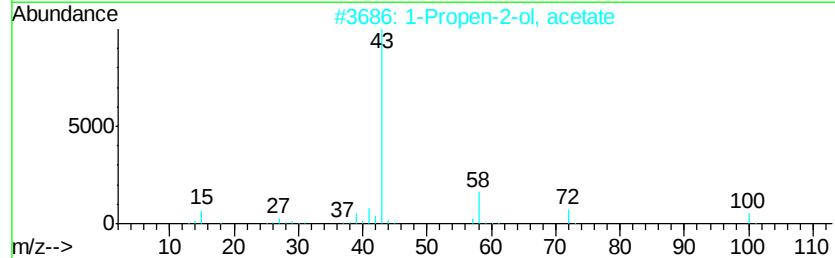
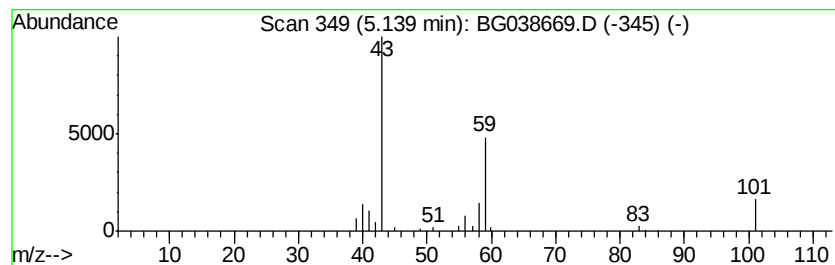
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	5.29 ng	38395	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
5		Diacetamide	101	C4H7NO2	000625-77-4	7



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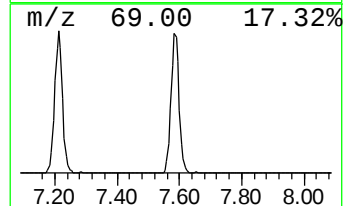
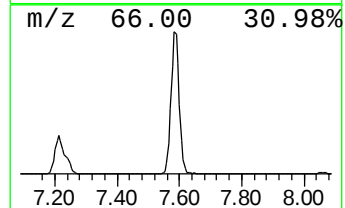
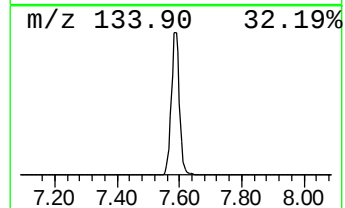
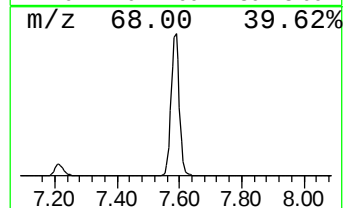
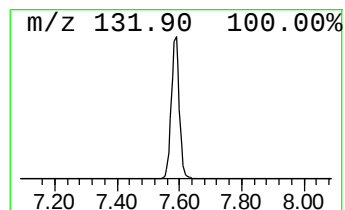
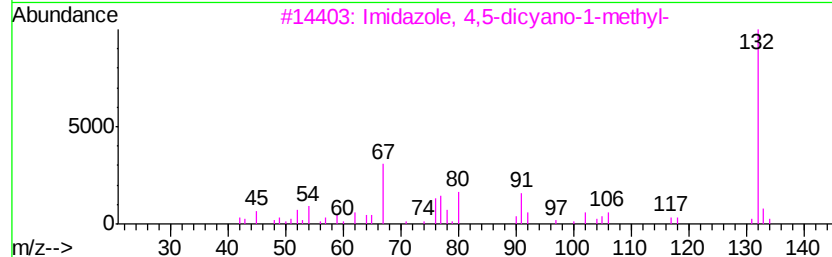
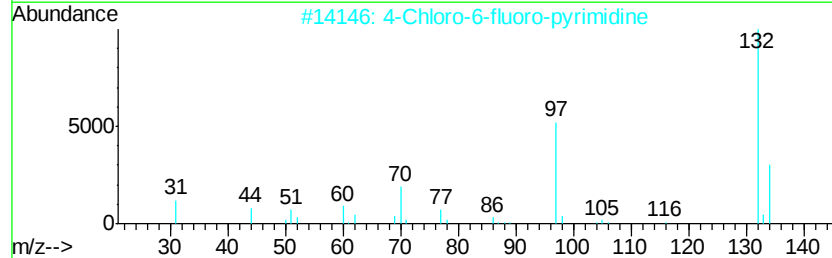
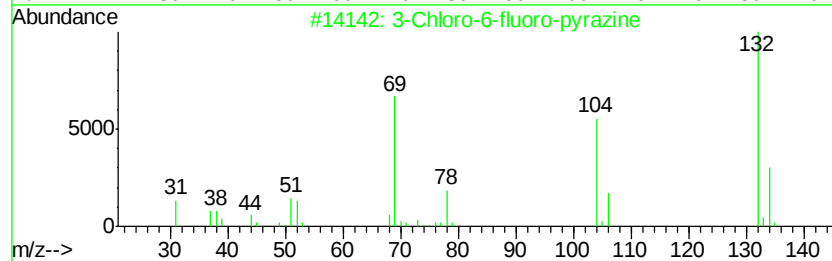
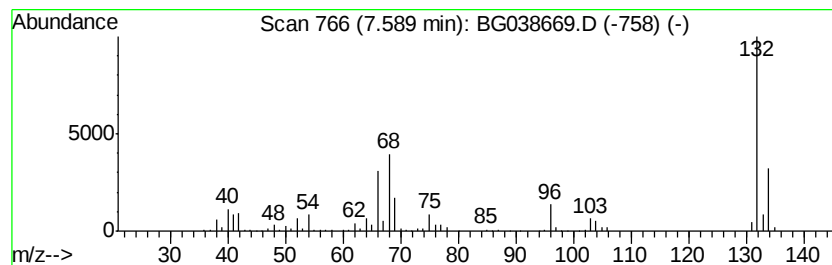
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	94.40 ng	684849	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
5		5-Aminoindole	132	C8H8N2	005192-03-0	22



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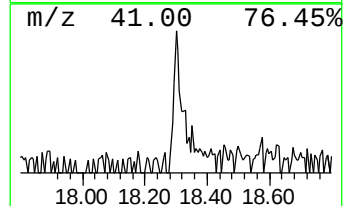
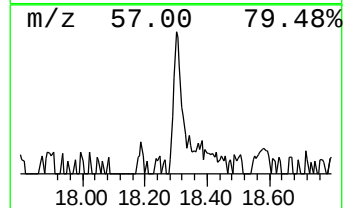
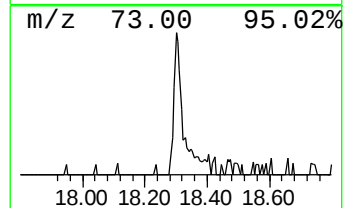
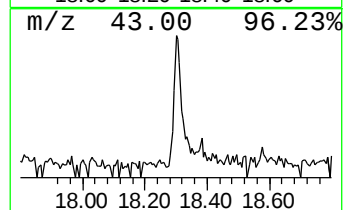
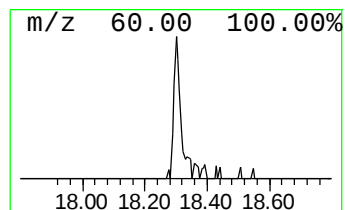
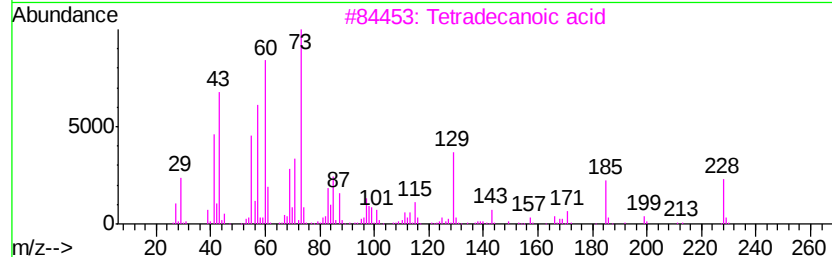
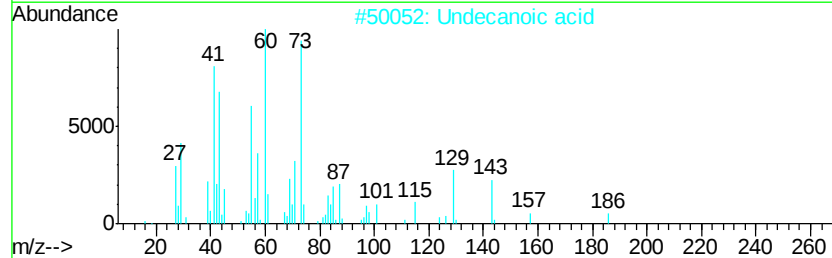
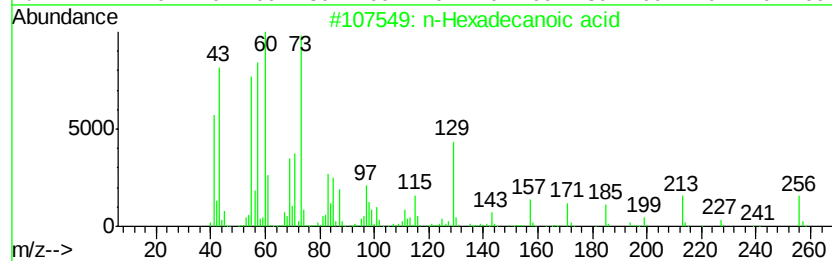
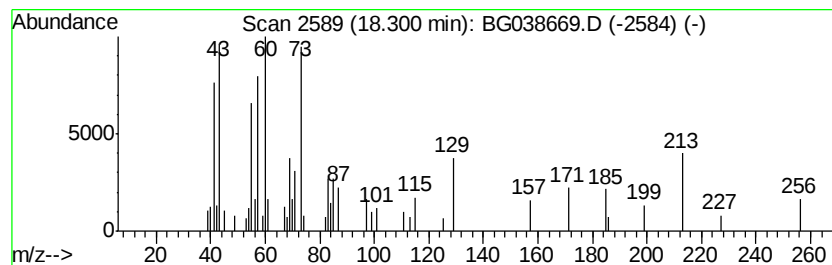
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.30	2.20 ng	42796	Phenanthrene-d10		17.44	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
2		Undecanoic acid	186	C11H22O2	000112-37-8	60
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Tridecanoic acid	214	C13H26O2	000638-53-9	52
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	47



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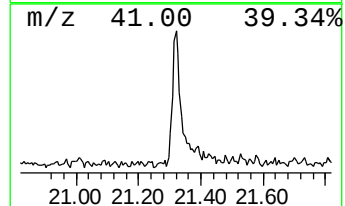
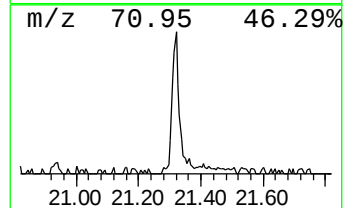
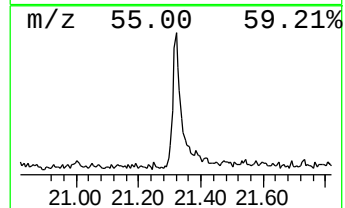
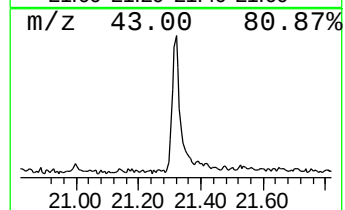
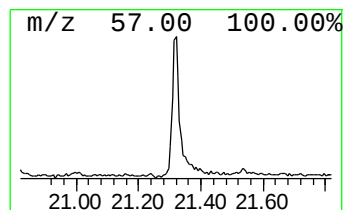
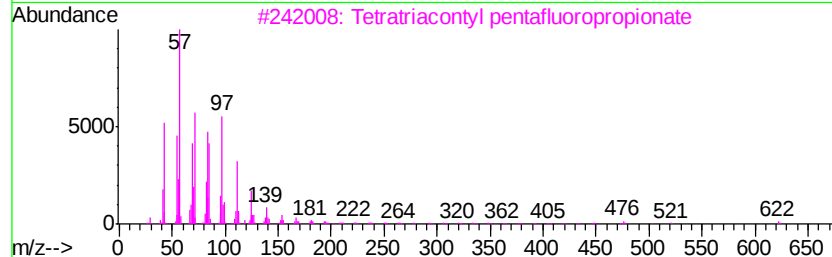
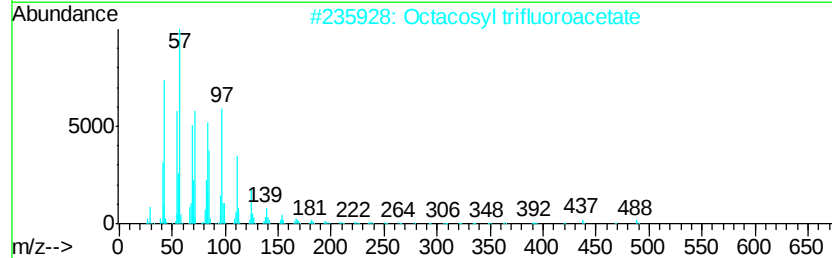
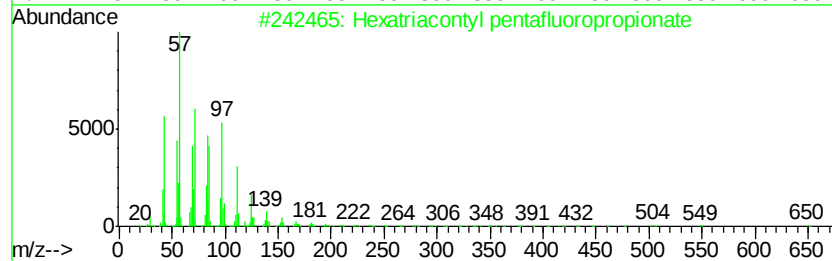
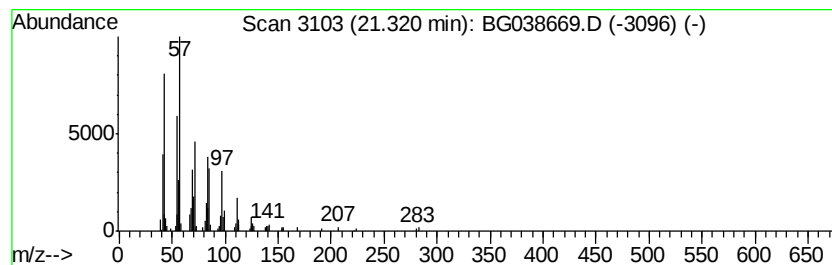
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Hexatriacontyl pentafluorop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	6.34 ng	145091	Chrysene-d12	21.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	91
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3		Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	91
4		Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	91
5		Triacetyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91



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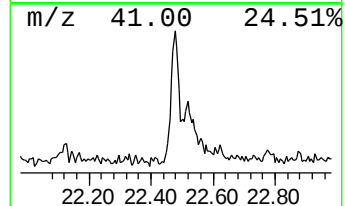
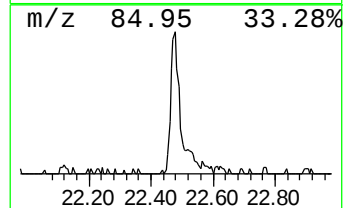
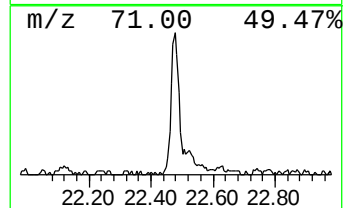
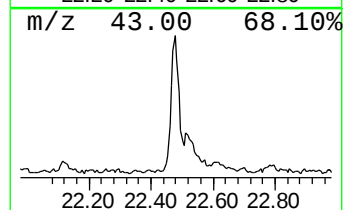
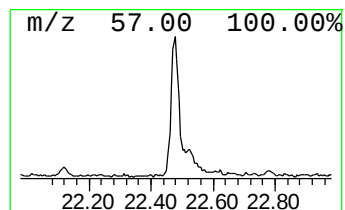
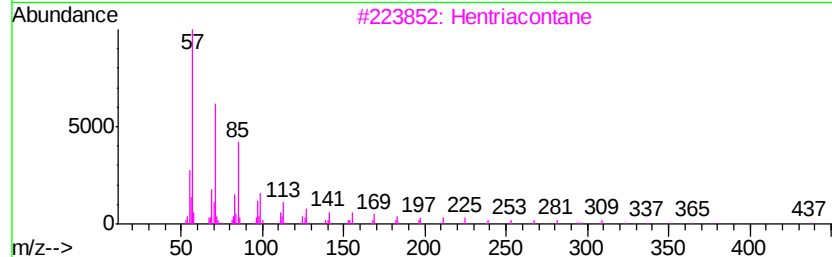
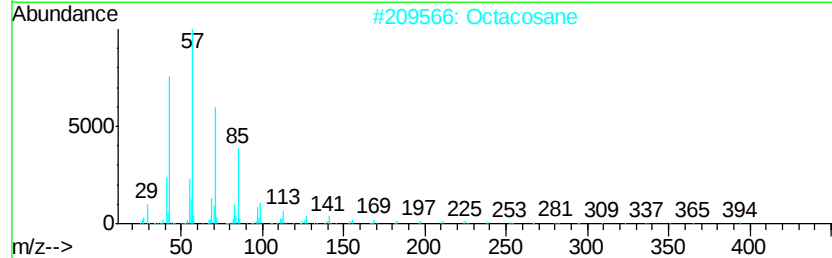
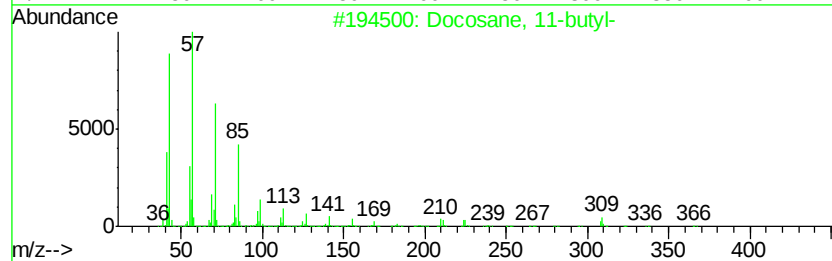
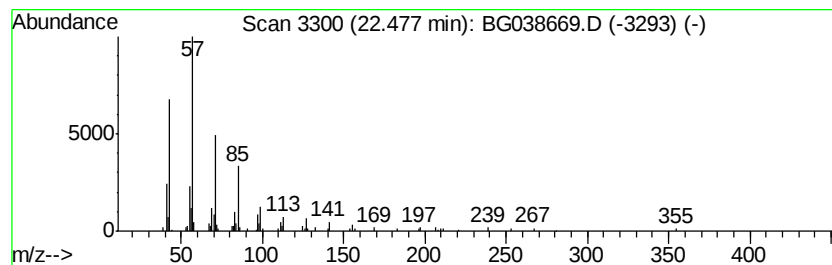
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Peak Number 6 Docosane, 11-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	5.25 ng	120054	Chrysene-d12	21.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-		366	C26H54	013475-76-8	90
2	Octacosane		394	C28H58	000630-02-4	90
3	Hentriacontane		437	C31H64	000630-04-6	87
4	Heneicosane		296	C21H44	000629-94-7	87
5	Tetracosane, 11-decyl-		479	C34H70	055429-84-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038669.D
Acq On : 17 Dec 2018 19:02
Operator : JU/SJ
Sample : J6391-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

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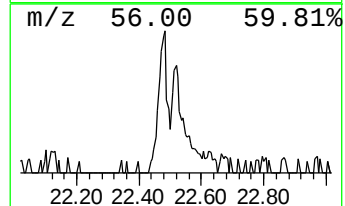
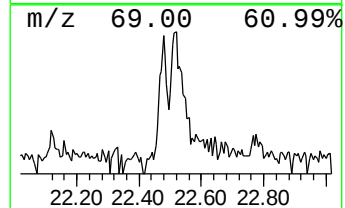
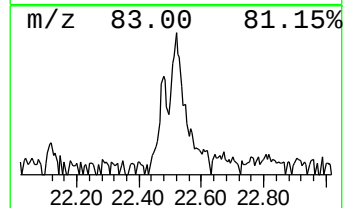
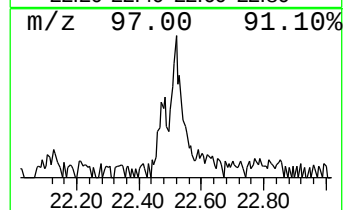
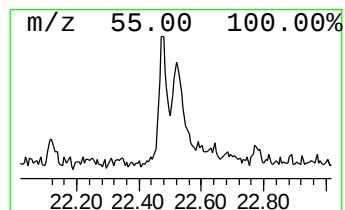
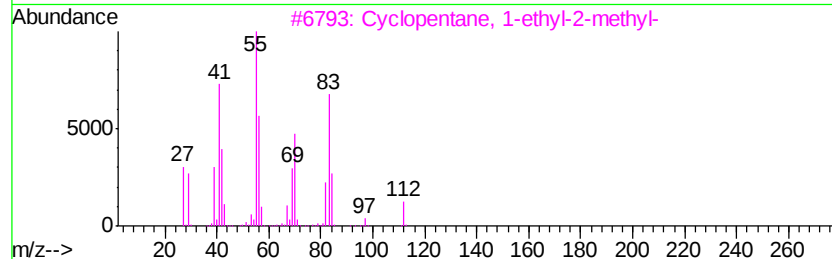
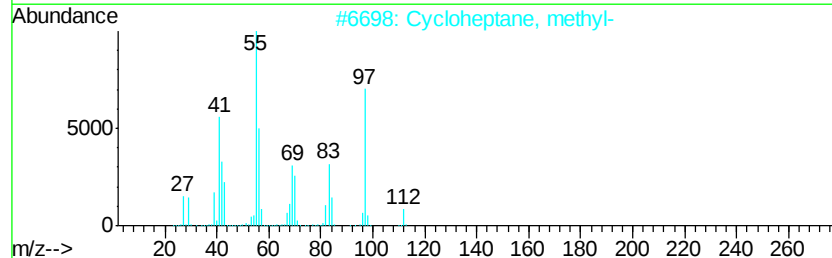
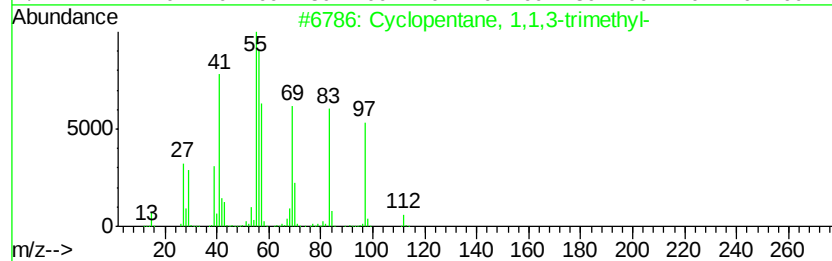
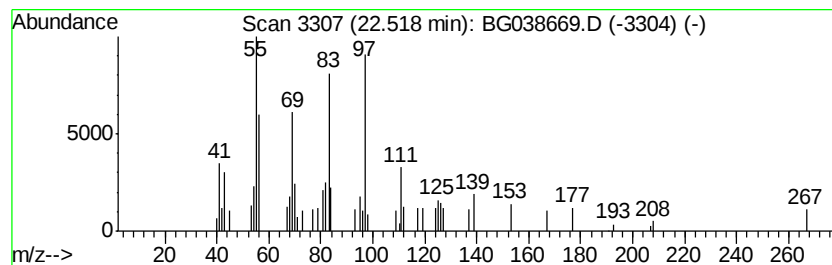
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.52	2.98 ng	68225	Chrysene-d12	21.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	70
2		Cycloheptane, methyl-	112	C8H16	004126-78-7	60
3		Cyclopentane, 1-ethyl-2-methyl-	112	C8H16	003726-46-3	38
4		Cyclopentane, 1-ethyl-3-methyl-,...	112	C8H16	002613-65-2	30
5		5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
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Sample : J6391-12
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ALS Vial : 17 Sample Multiplier: 1

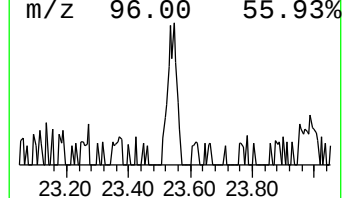
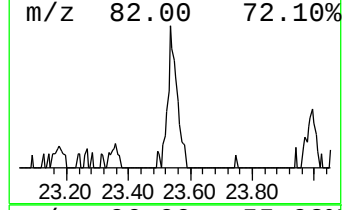
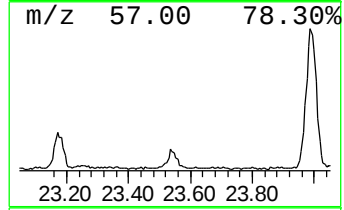
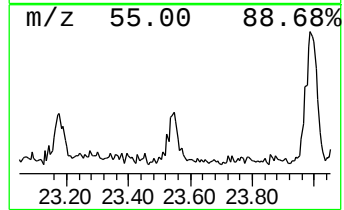
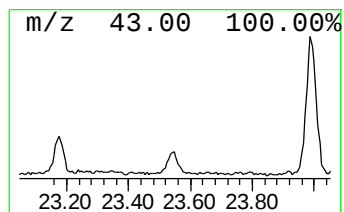
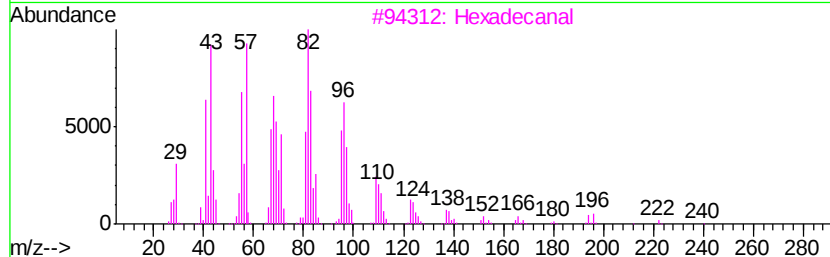
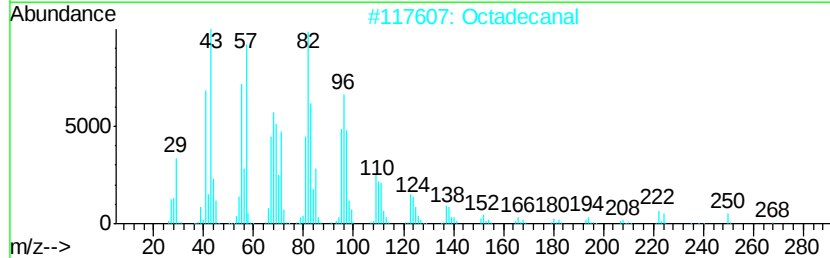
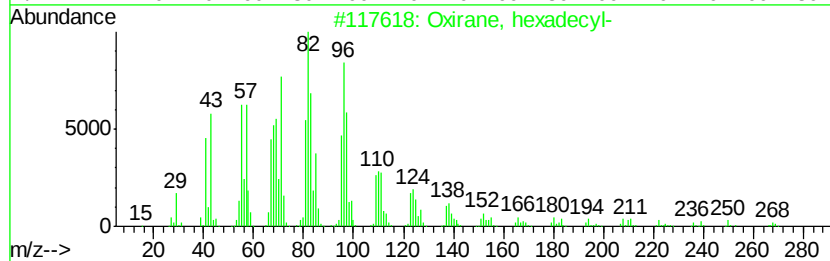
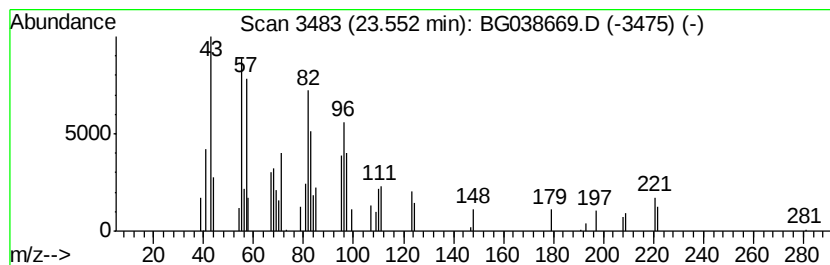
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.55	2.19 ng	45694	Perylene-d12	25.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
2	Octadecanal	268	C18H36O	000638-66-4	87
3	Hexadecanal	240	C16H32O	000629-80-1	83
4	Pentadecanal-	226	C15H30O	002765-11-9	81
5	1,19-Eicosadiene	278	C20H38	014811-95-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038669.D
Acq On : 17 Dec 2018 19:02
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Instrument :
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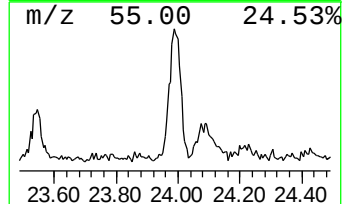
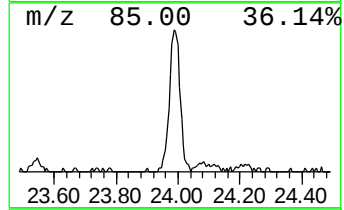
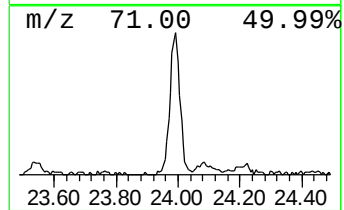
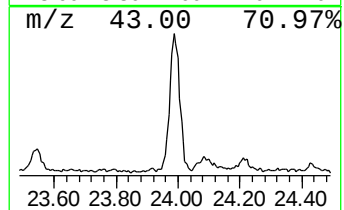
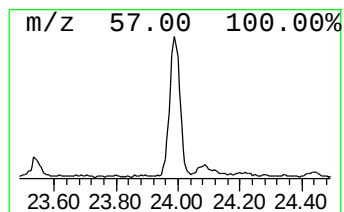
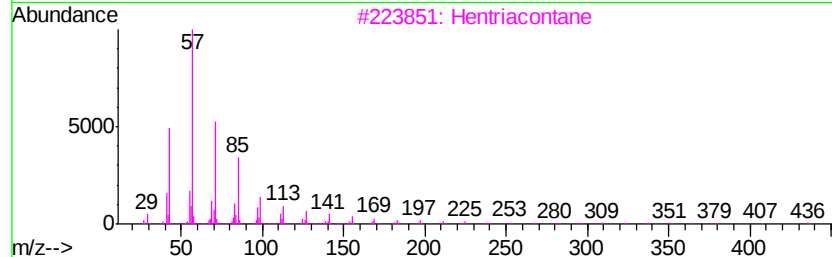
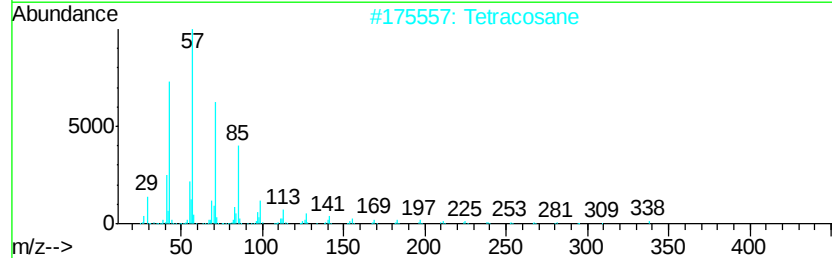
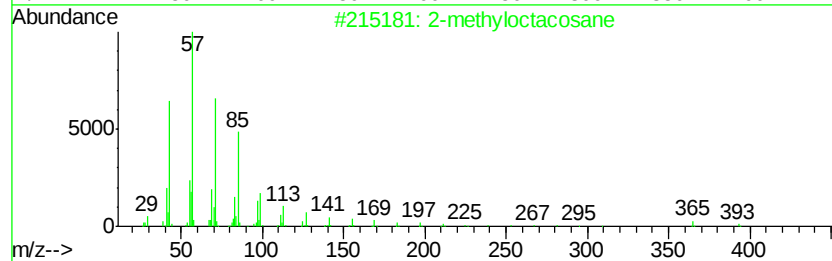
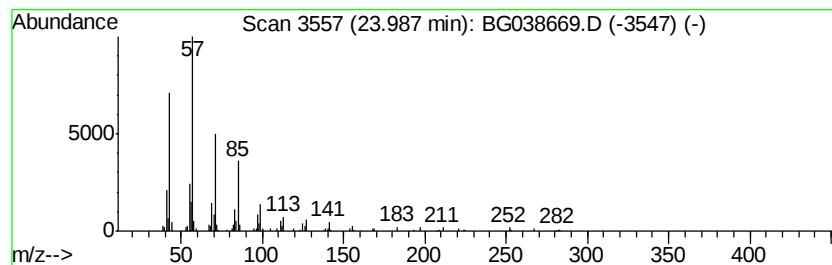
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	10.13 ng	210820	Perylene-d12	25.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	91
2	Tetracosane		338	C24H50	000646-31-1	90
3	Hentriacontane		437	C31H64	000630-04-6	90
4	Hexatriacontane		507	C36H74	000630-06-8	90
5	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
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Acq On : 17 Dec 2018 19:02
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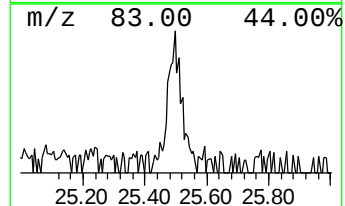
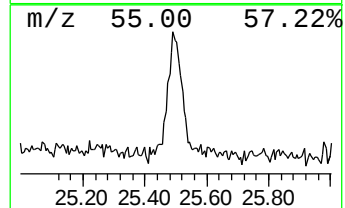
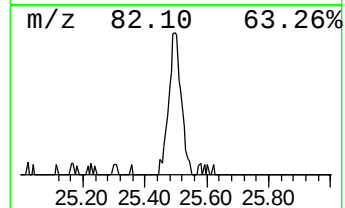
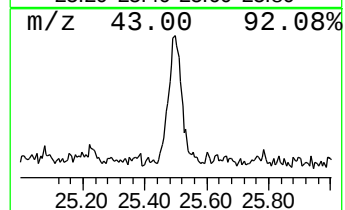
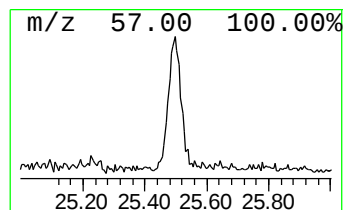
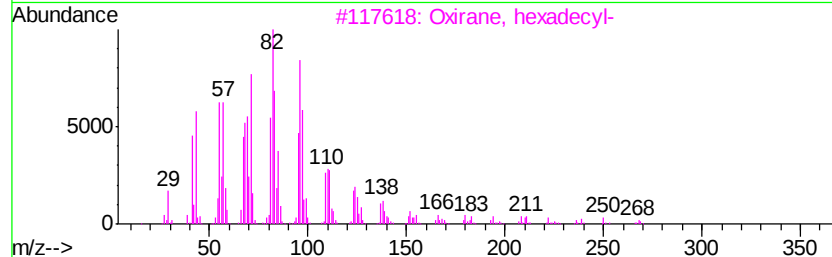
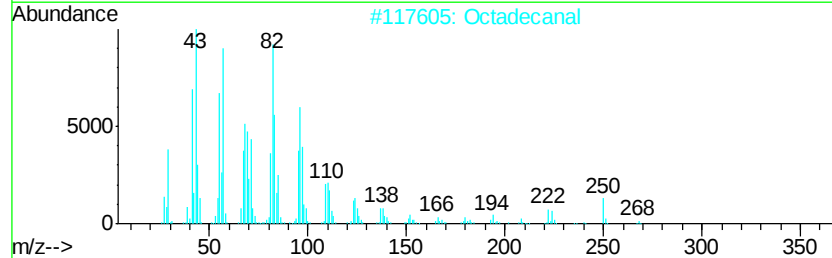
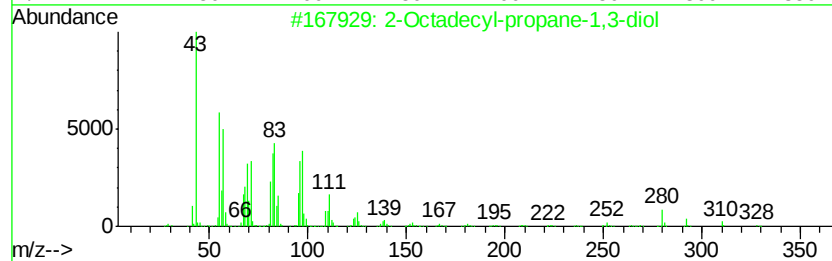
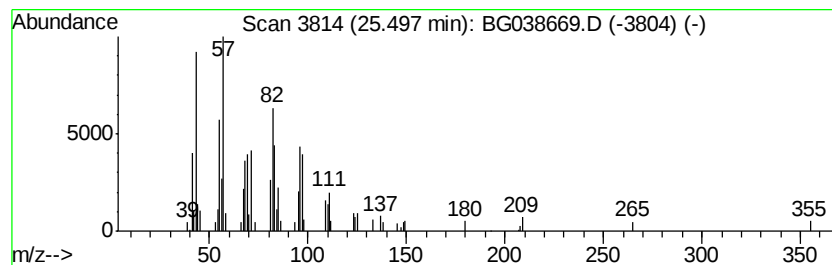
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Octadecyl-propane-1,3-diol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
25.50	5.10 ng	106178	Perylene-d12		25.02
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	80
2	Octadecanal	268	C18H36O	000638-66-4	64
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	59
4	17-Pentatriacontene	491	C35H70	006971-40-0	58
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038669.D
Acq On : 17 Dec 2018 19:02
Operator : JU/SJ
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ClientSampleId :
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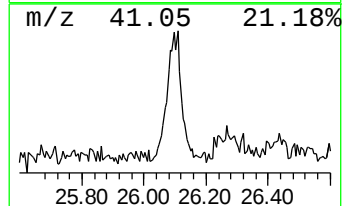
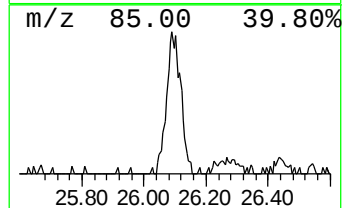
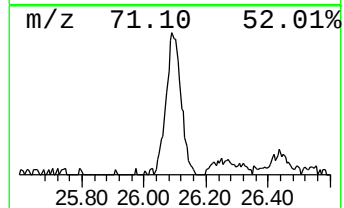
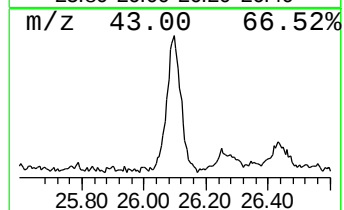
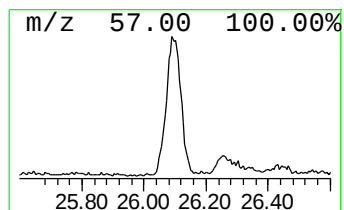
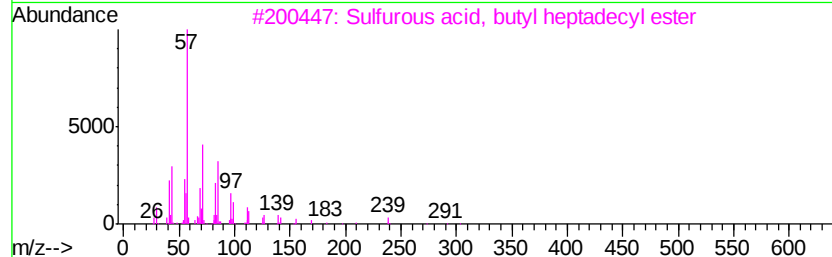
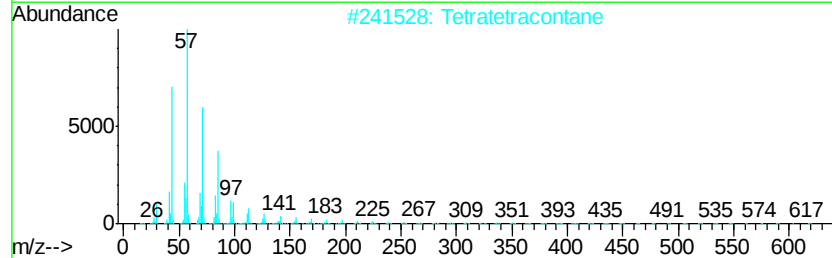
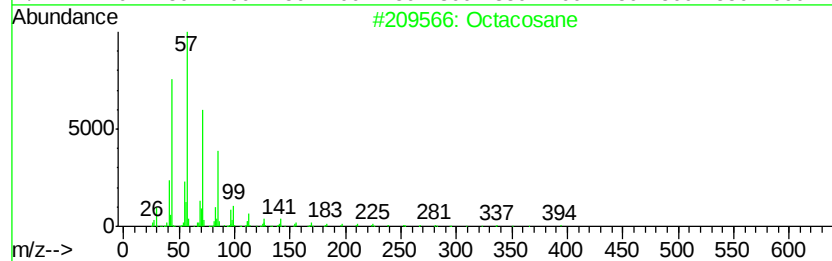
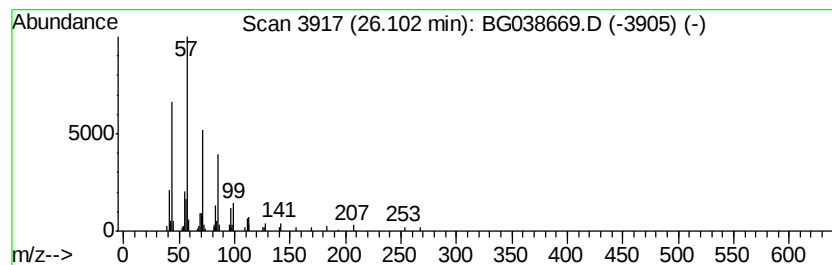
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.10	6.76 ng	140685	Perylene-d12	25.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	87
4		Hentriacontane	437	C31H64	000630-04-6	86
5		Hexatriacontane	507	C36H74	000630-06-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038669.D
Acq On : 17 Dec 2018 19:02
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ClientSampleId :
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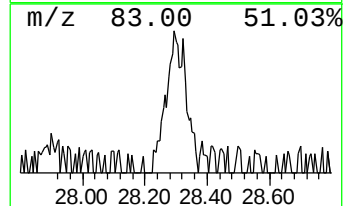
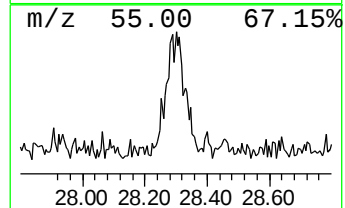
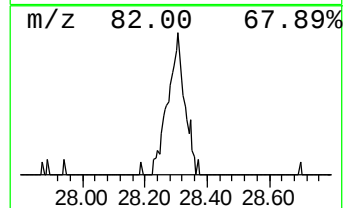
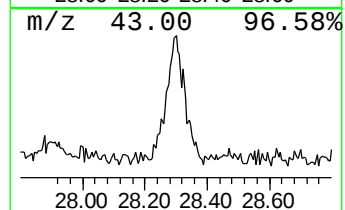
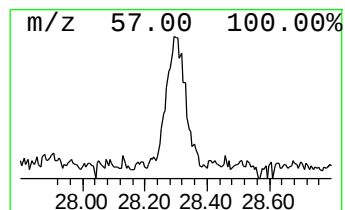
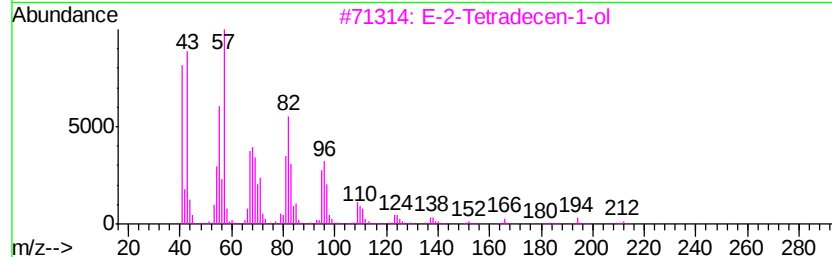
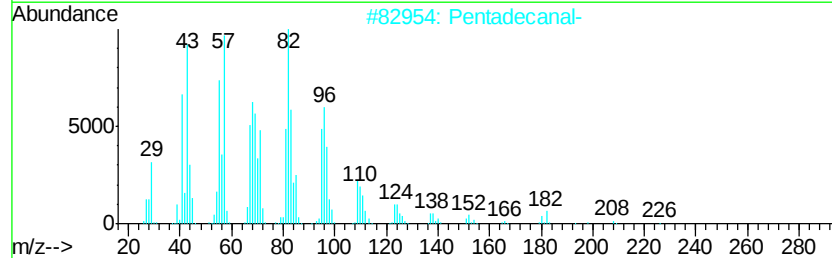
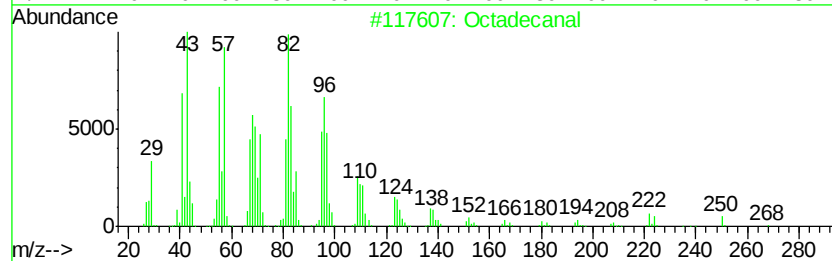
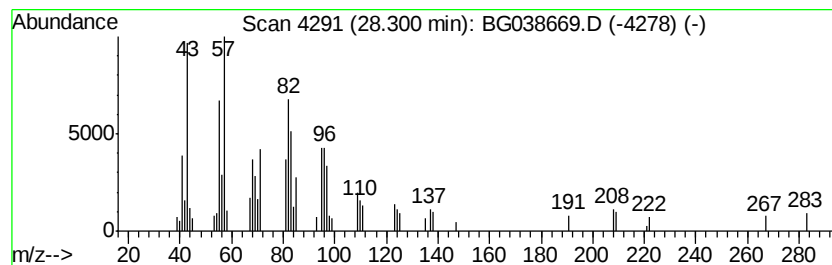
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.30	4.68 ng	97425	Perylene-d12	25.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	90
2			Pentadecanal-	226	C15H30O	002765-11-9	86
3			E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	86
4			Heptadecanal	254	C17H34O	1000376-70-0	81
5			Hexadecanal	240	C16H32O	000629-80-1	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
 Data File : BG038669.D
 Acq On : 17 Dec 2018 19:02
 Operator : JU/SJ
 Sample : J6391-12
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 ALS Vial : 17 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown7.59	7.59	94.4	ng	684849	1	8.06	145091	20.0
n-Hexadecanoic acid	18.30	2.2	ng	42796	4	17.44	389774	20.0
Hexatriacontyl pe...	21.32	6.3	ng	145091	5	21.72	457401	20.0
Docosane, 11-butyl-	22.48	5.3	ng	120054	5	21.72	457401	20.0
Cyclopentane, 1,1...	22.52	3.0	ng	68225	5	21.72	457401	20.0
Oxirane, hexadecyl-	23.55	2.2	ng	45694	6	25.02	416414	20.0
2-methyloctacosane	23.99	10.1	ng	210820	6	25.02	416414	20.0
2-Octadecyl-propa...	25.50	5.1	ng	106178	6	25.02	416414	20.0
Octacosane	26.10	6.8	ng	140685	6	25.02	416414	20.0
Octadecanal	28.30	4.7	ng	97425	6	25.02	416414	20.0