

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
 Data File : BG038671.D
 Acq On : 17 Dec 2018 20:21
 Operator : JU/SJ
 Sample : J6347-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P001-SD001-0612-01

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	5.143	346	350	359	rVB2	24360	40942	2.63%	0.402%
2	5.607	422	429	435	rBV	433259	712864	45.73%	7.004%
3	5.672	435	440	450	rVB	204949	415369	26.64%	4.081%
4	6.048	498	504	513	rBV2	57000	96359	6.18%	0.947%
5	7.211	694	702	720	rVB	451581	837917	53.75%	8.233%
6	7.587	758	766	776	rBV	410167	738260	47.36%	7.254%
7	8.058	839	846	857	rBV2	74333	147627	9.47%	1.451%
8	8.381	894	901	910	rVB	303197	540724	34.69%	5.313%
9	9.239	1037	1047	1058	rBV	261935	498100	31.95%	4.894%
10	10.878	1319	1326	1332	rBV	96840	179674	11.53%	1.765%
11	13.316	1732	1741	1751	rBV	664291	1049711	67.34%	10.314%
12	14.139	1876	1881	1888	rBV	43757	64369	4.13%	0.632%
13	14.697	1969	1976	1985	rVB2	164131	269425	17.28%	2.647%
14	16.183	2222	2229	2243	rBV	615617	961330	61.67%	9.446%
15	17.441	2437	2443	2456	rBV	232412	369281	23.69%	3.628%
16	18.304	2584	2590	2600	rBV2	42808	73044	4.69%	0.718%
17	19.573	2801	2806	2810	rBV4	9780	15822	1.01%	0.155%
18	20.043	2880	2886	2892	rBV	1169903	1558919	100.00%	15.317%
19	20.314	2926	2932	2936	rBV5	9759	16358	1.05%	0.161%
20	21.318	3097	3103	3117	rBV	104586	183158	11.75%	1.800%
21	21.724	3163	3172	3181	rBV2	240653	408314	26.19%	4.012%
22	21.847	3186	3193	3202	rBV5	11524	30875	1.98%	0.303%
23	22.476	3293	3300	3304	rBV	49048	91678	5.88%	0.901%
24	22.517	3304	3307	3321	rVB8	21999	65084	4.17%	0.639%
25	23.157	3409	3416	3425	rBV7	17743	53366	3.42%	0.524%
26	23.375	3447	3453	3462	rVB5	11258	25059	1.61%	0.246%
27	23.992	3550	3558	3565	rBV	34210	80519	5.17%	0.791%
28	25.020	3723	3733	3744	rVB2	131815	388225	24.90%	3.815%
29	25.502	3804	3815	3824	rBV6	17968	51194	3.28%	0.503%
30	26.289	3928	3949	3950	rBV7	33011	129905	8.33%	1.276%
31	28.304	4279	4292	4307	rBV8	19457	83928	5.38%	0.825%

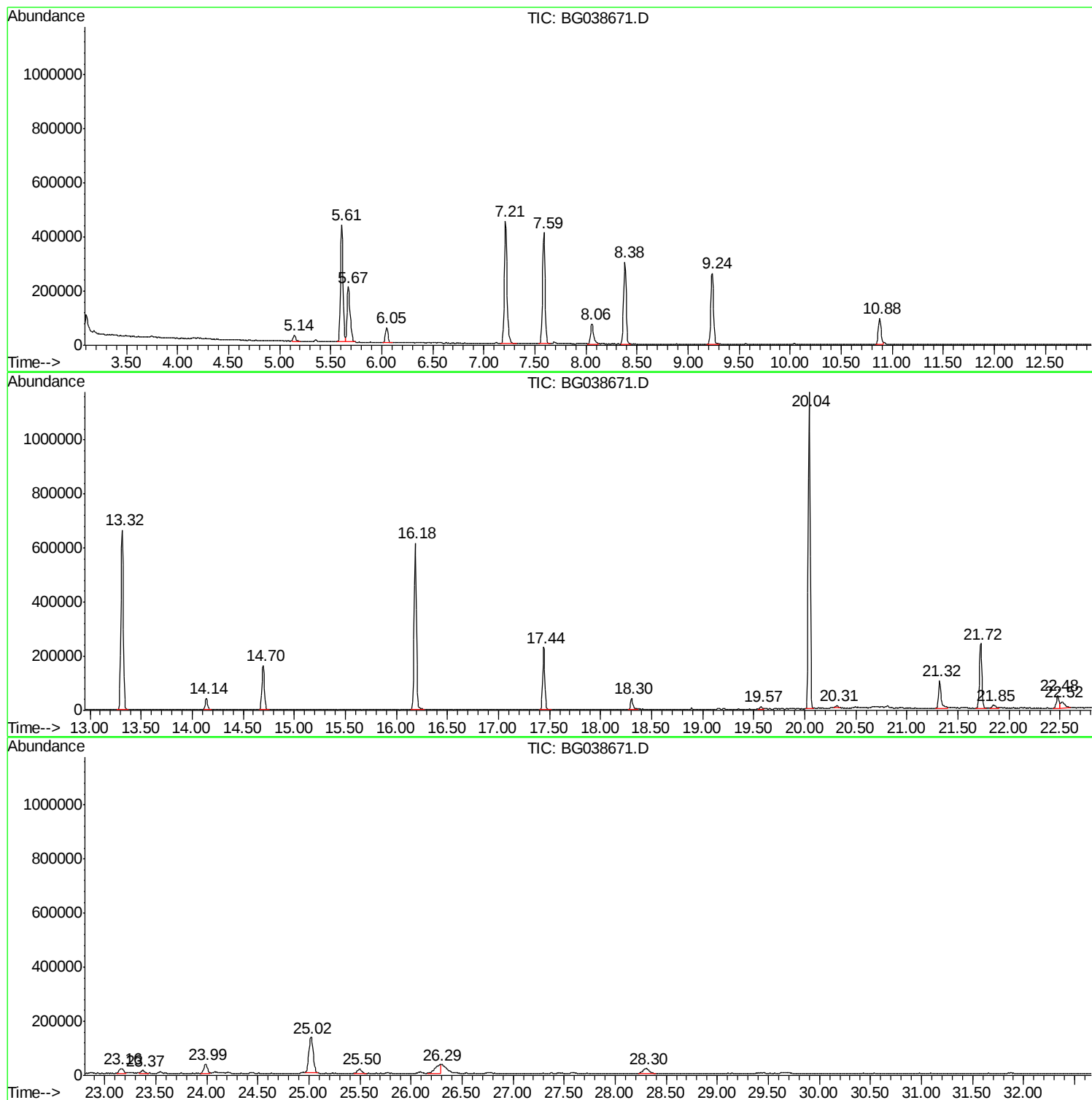
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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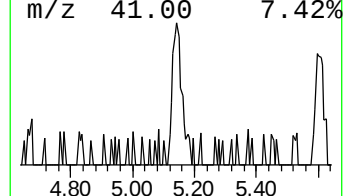
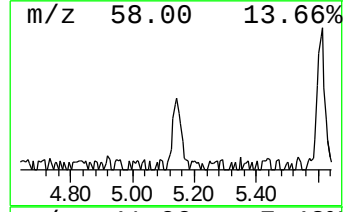
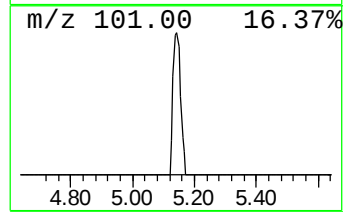
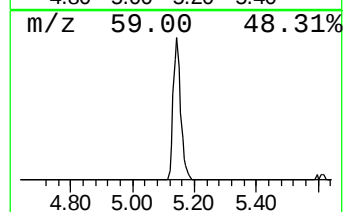
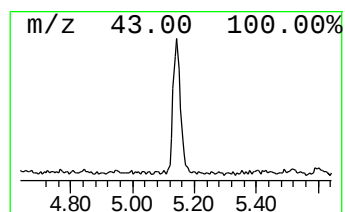
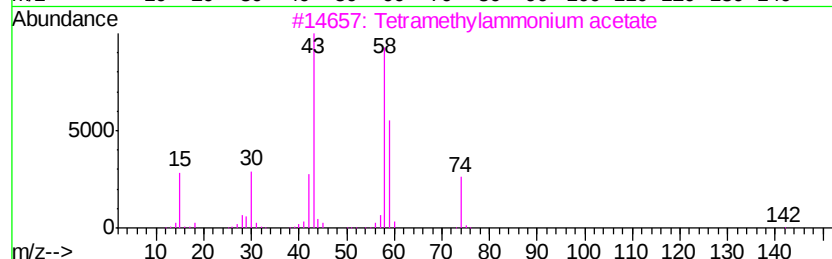
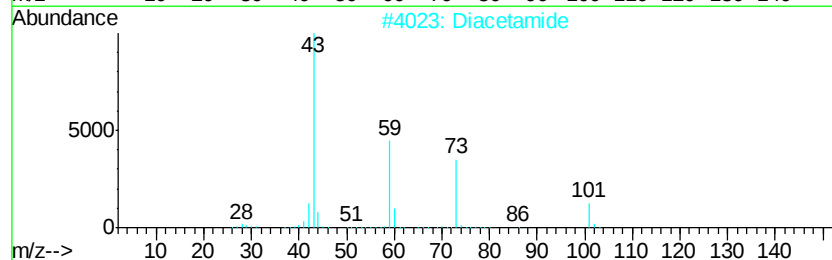
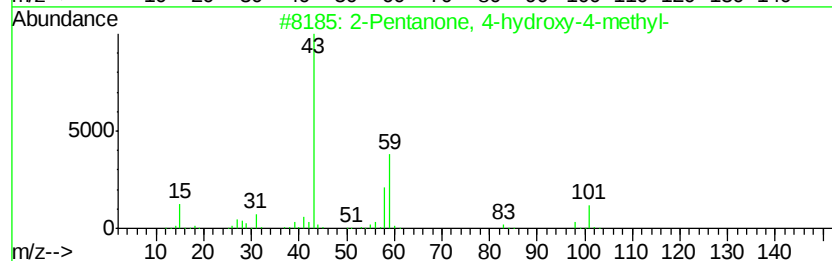
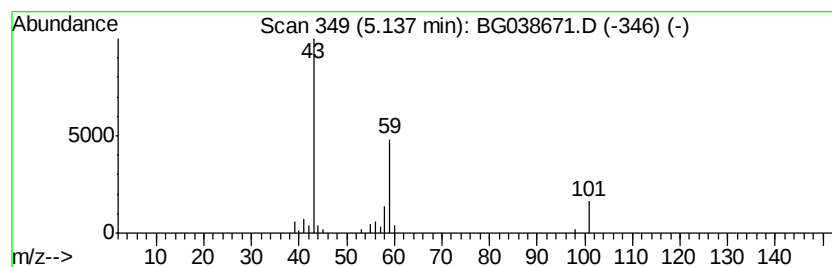
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	5.55 ng	40942	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	64
2		Diacetamide	101	C4H7NO2	000625-77-4	9
3		Tetramethylammonium acetate	133	C6H15N02	010581-12-1	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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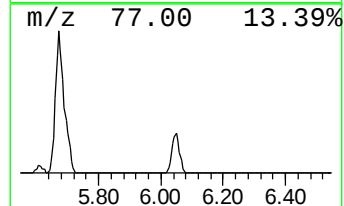
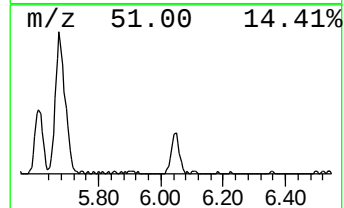
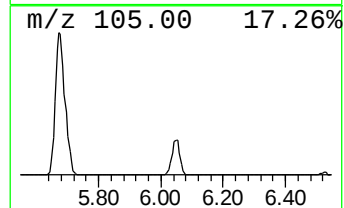
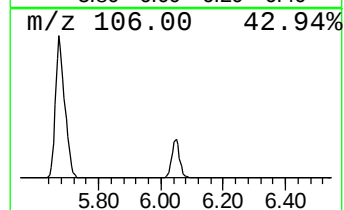
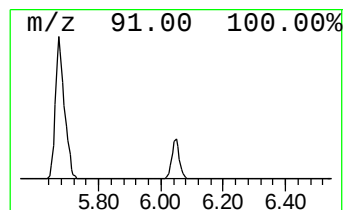
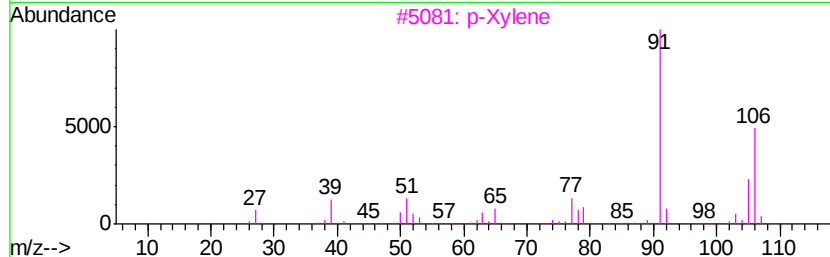
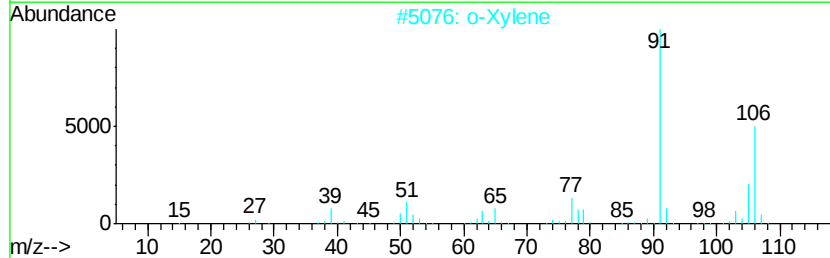
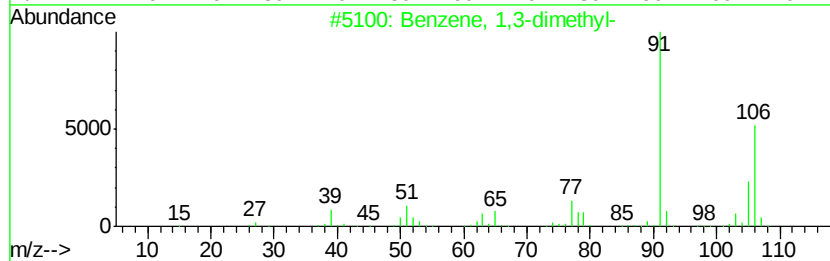
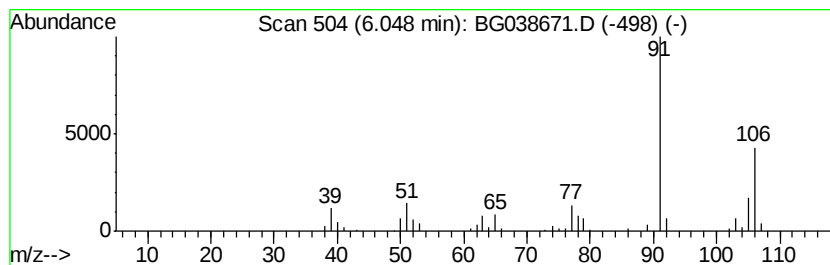
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Peak Number 3 Benzene, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.05	13.05 ng	96359	1,4-Dichlorobenzene-d4	8.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2			o-Xylene	106	C8H10	000095-47-6	97
3			p-Xylene	106	C8H10	000106-42-3	95
4			Ethylbenzene	106	C8H10	000100-41-4	93
5			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	87



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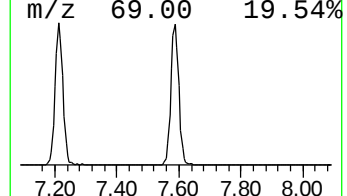
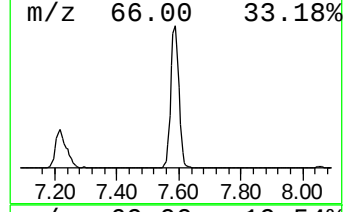
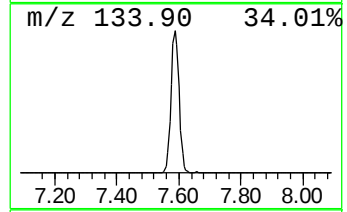
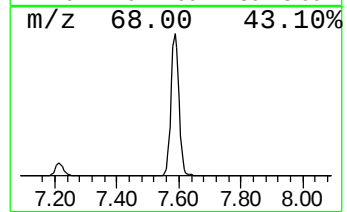
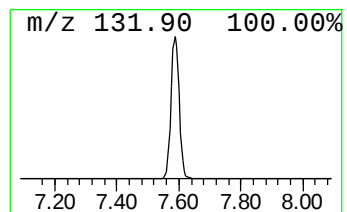
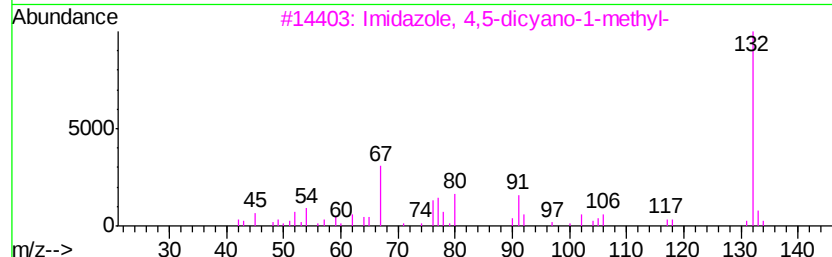
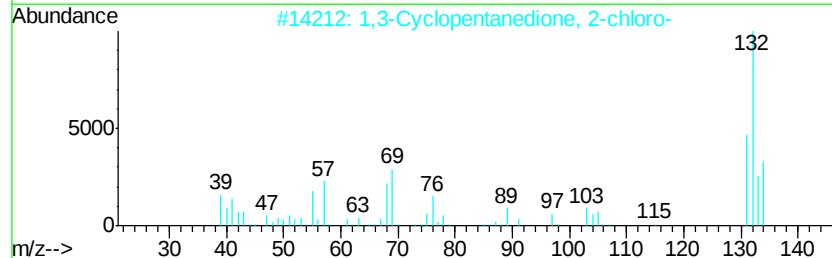
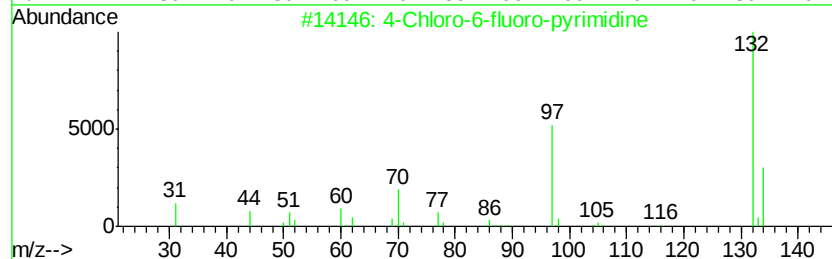
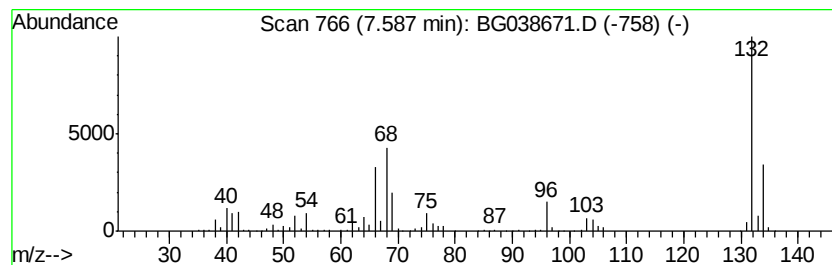
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Peak Number 4 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	100.02 ng	738260	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		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



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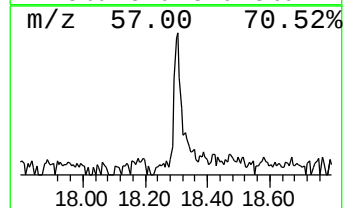
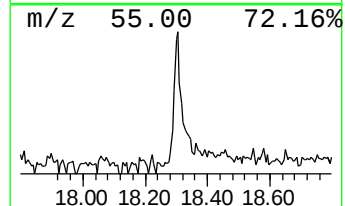
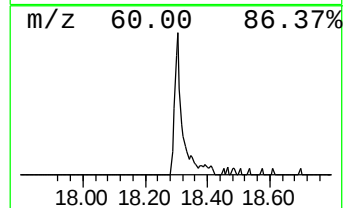
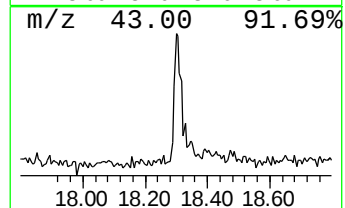
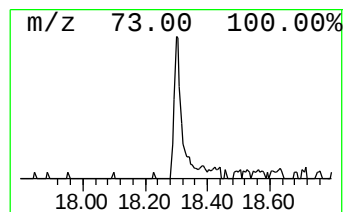
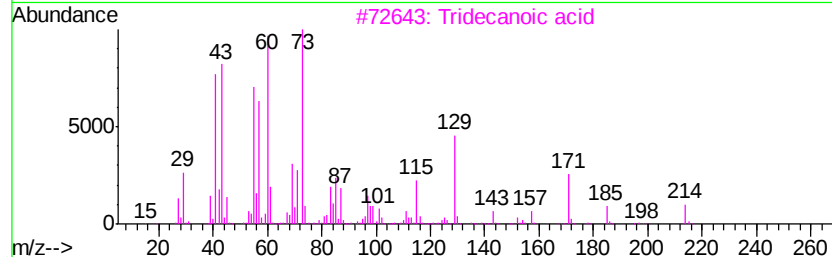
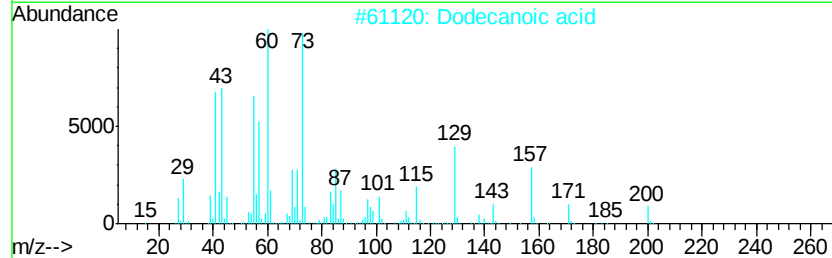
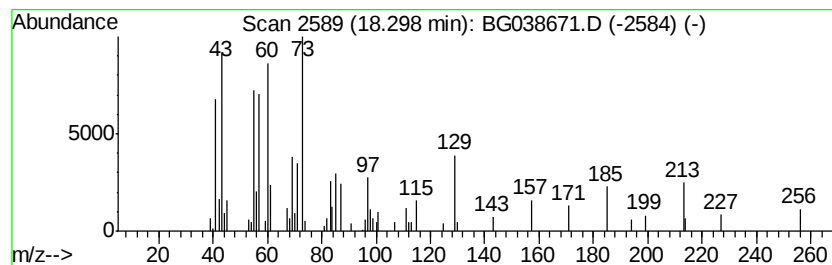
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.30	3.96 ng	73044	Phenanthrene-d10		17.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Dodecanoic acid	200	C12H24O2	000143-07-7	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53



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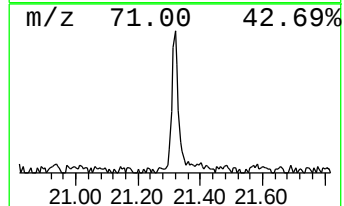
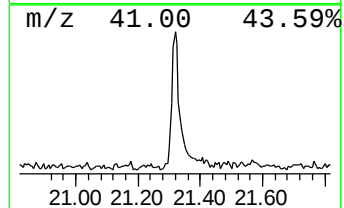
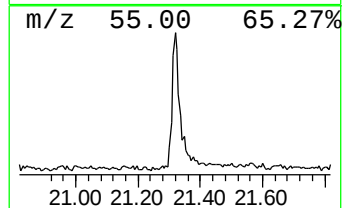
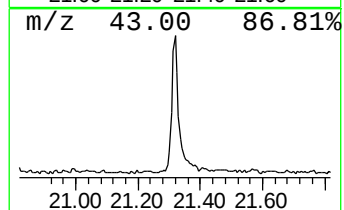
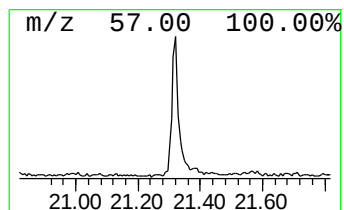
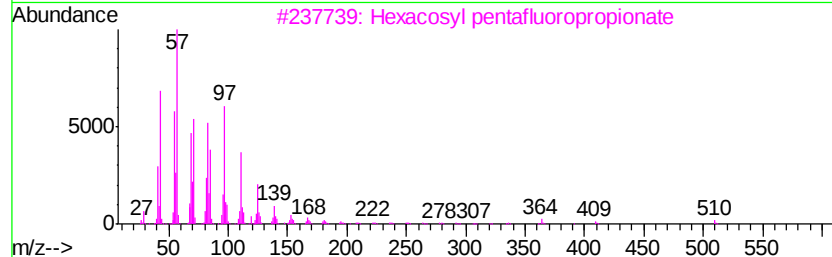
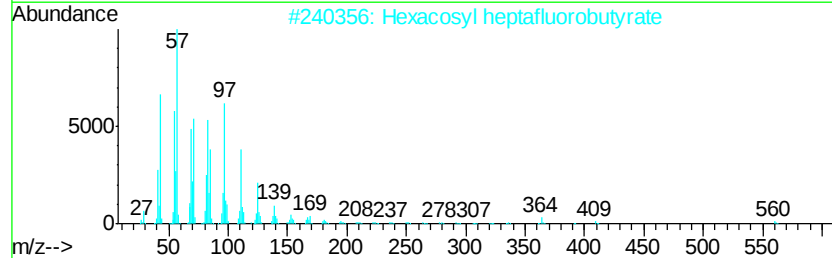
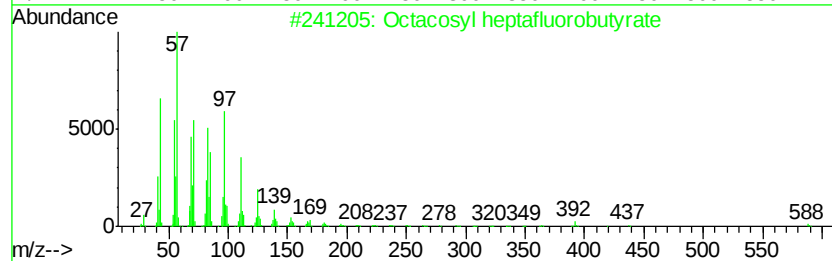
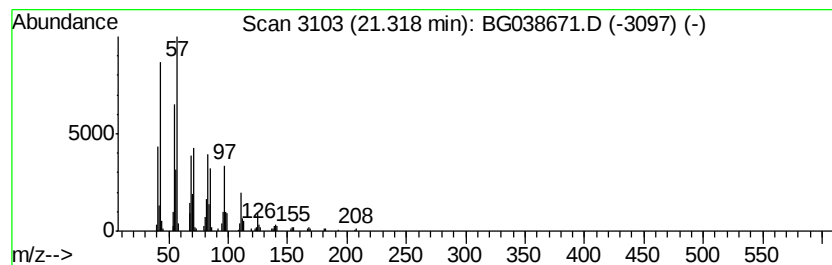
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Peak Number 7 Octacosyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	8.97 ng	183158	Chrysene-d12	21.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91
2		Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
3		Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
4		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
5		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91



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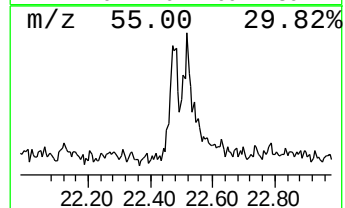
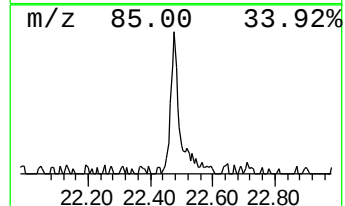
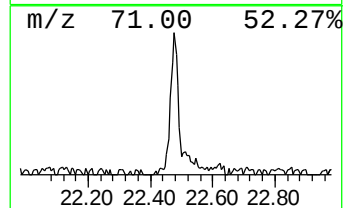
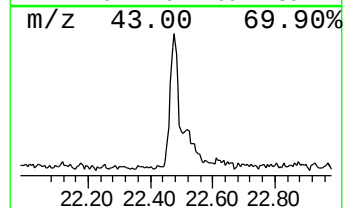
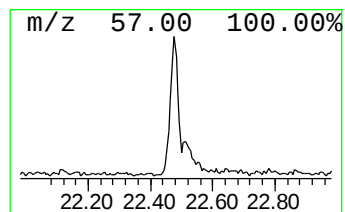
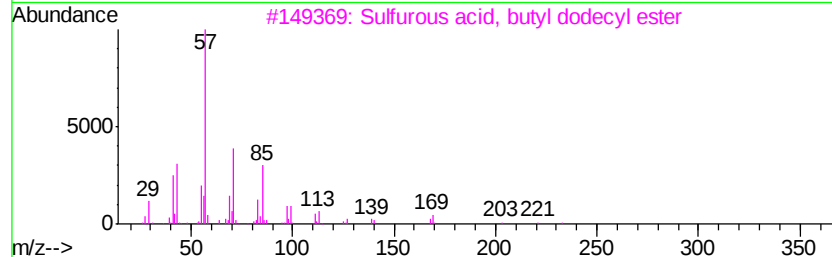
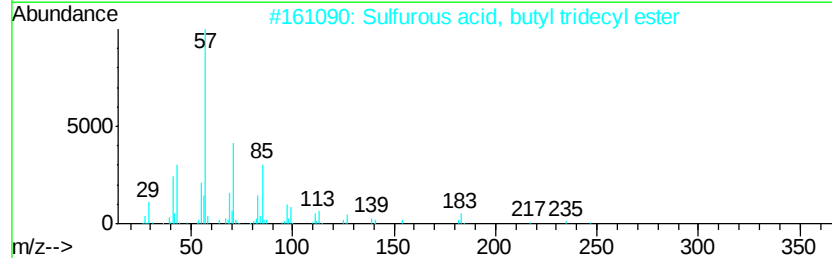
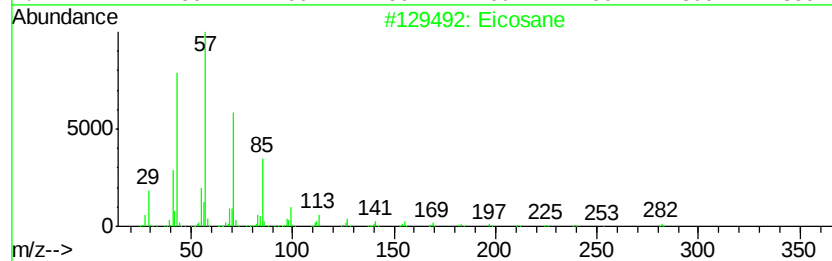
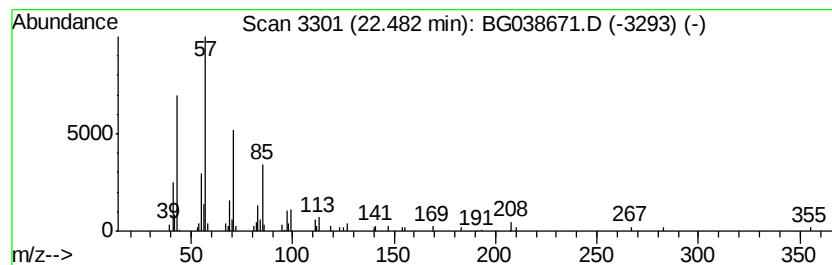
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
22.48	4.49 ng	91678	Chrysene-d12	21.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	96
2	Sulfurous acid, butyl tridecyl e...		320	C17H36O3S	1000309-18-0	90
3	Sulfurous acid, butyl dodecyl ester		306	C16H34O3S	1000309-17-9	90
4	Tetracosane		338	C24H50	000646-31-1	87
5	Heneicosane		296	C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038671.D
Acq On : 17 Dec 2018 20:21
Operator : JU/SJ
Sample : J6347-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P001-SD001-0612-01

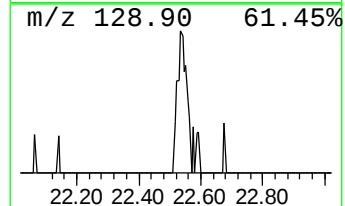
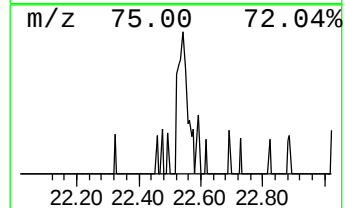
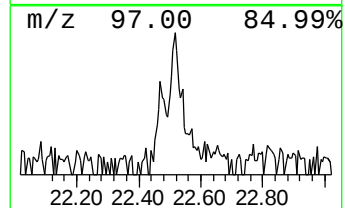
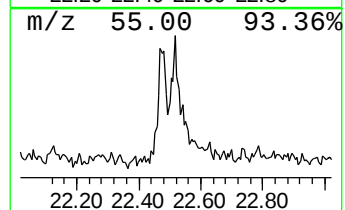
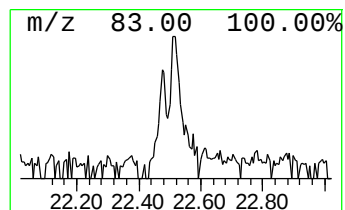
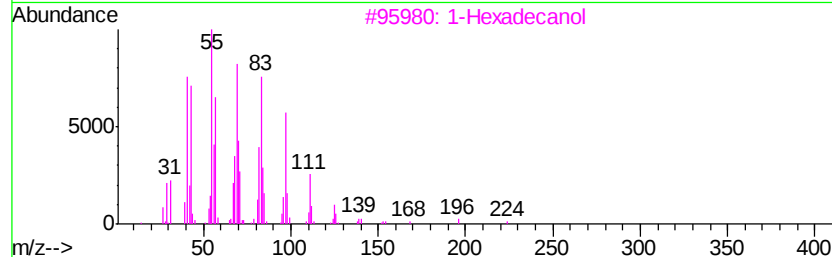
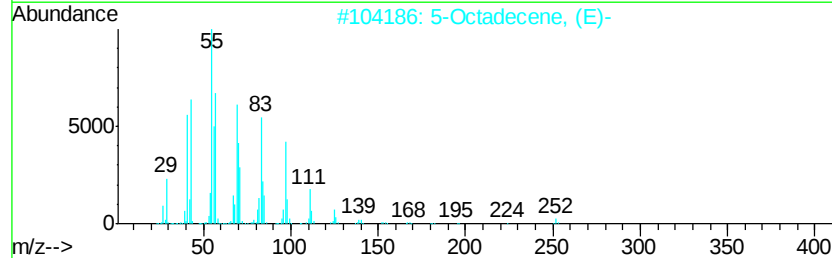
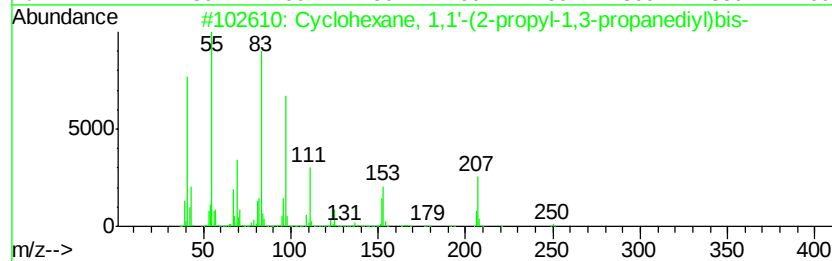
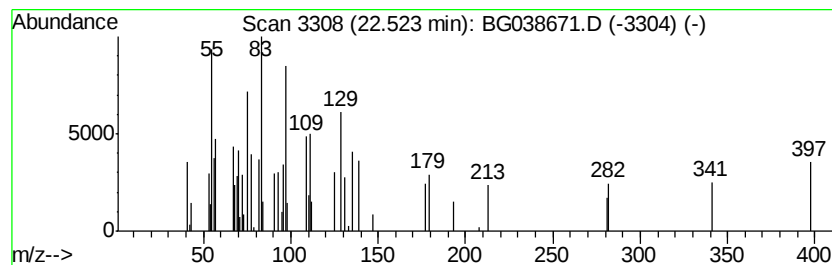
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown22.52 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.52	3.19 ng	65084	Chrysene-d12	21.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1'-(2-propyl-1,3-...	250	C18H34	055030-21-2	47
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	47
3		1-Hexadecanol	242	C16H34O	036653-82-4	43
4		Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	38
5		Cyclodecane, octyl-	252	C18H36	016539-09-6	37



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038671.D
Acq On : 17 Dec 2018 20:21
Operator : JU/SJ
Sample : J6347-03
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Instrument :
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ClientSampleId :
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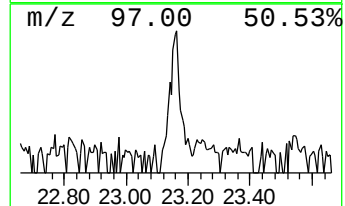
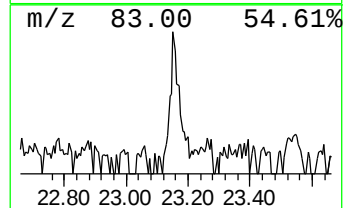
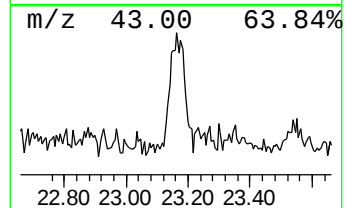
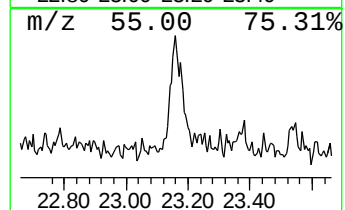
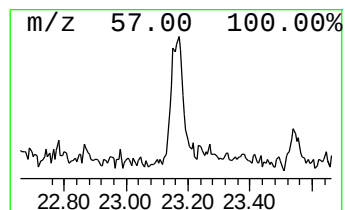
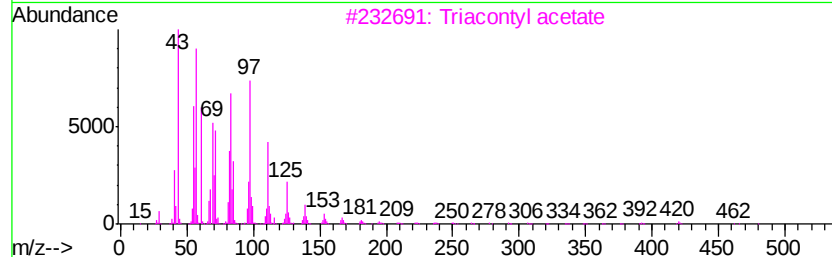
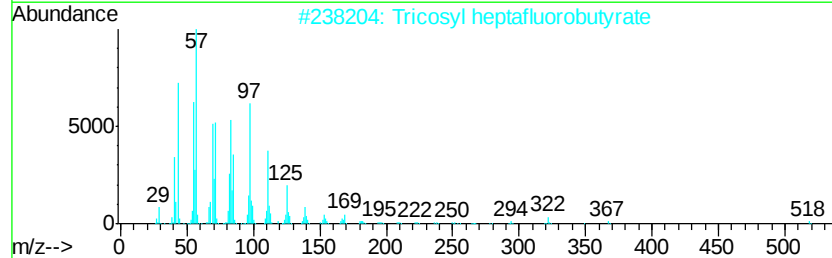
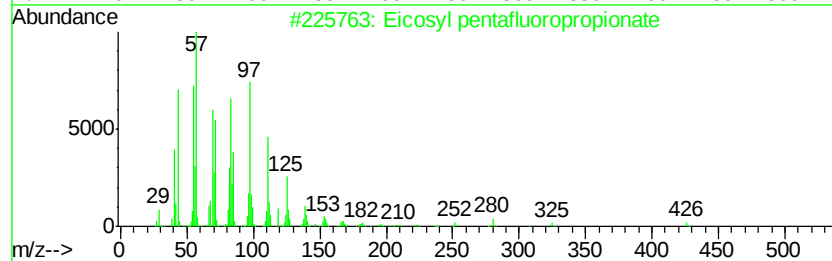
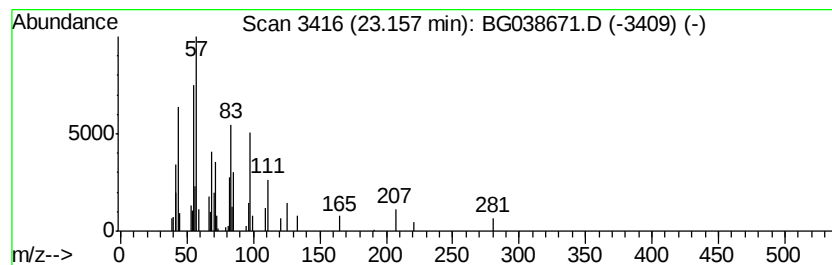
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosyl pentafluoropropionate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.16	2.61 ng	53366	Chrysene-d12	21.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	83
2			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	83
3			Triacontyl acetate	480	C32H64O2	041755-58-2	83
4			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	83
5			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038671.D
Acq On : 17 Dec 2018 20:21
Operator : JU/SJ
Sample : J6347-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P001-SD001-0612-01

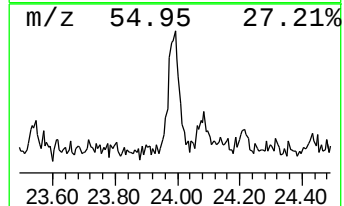
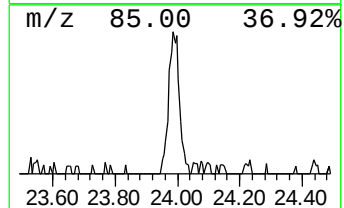
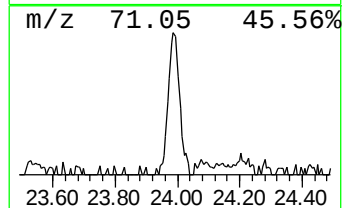
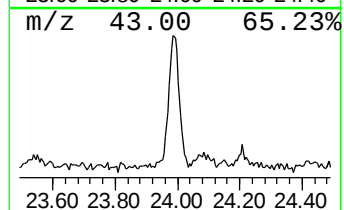
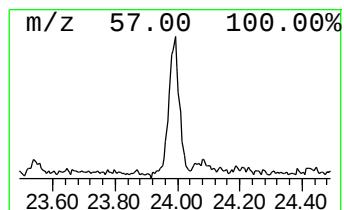
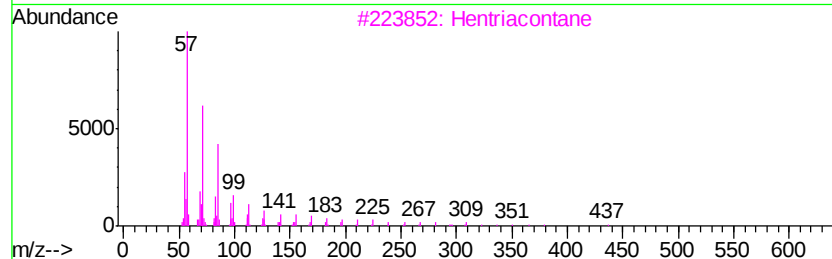
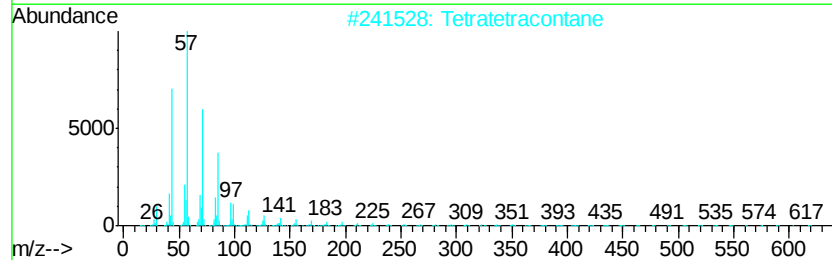
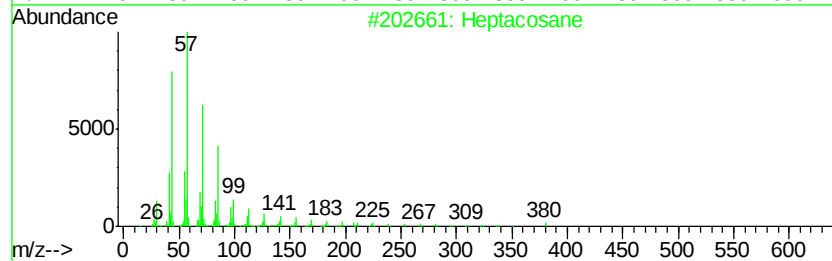
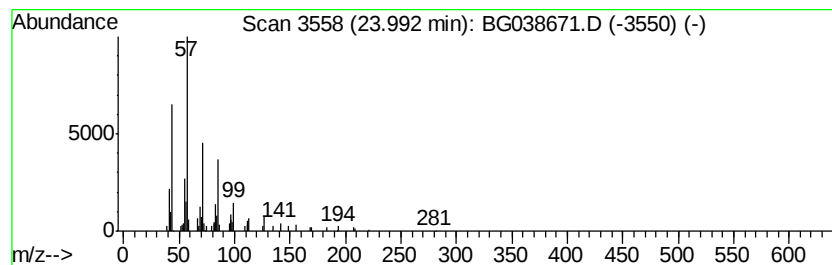
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	4.15 ng	80519	Perylene-d12	25.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Octacosane	394	C28H58	000630-02-4	87
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
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Acq On : 17 Dec 2018 20:21
Operator : JU/SJ
Sample : J6347-03
Misc :
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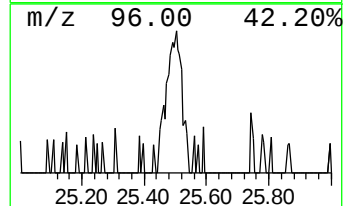
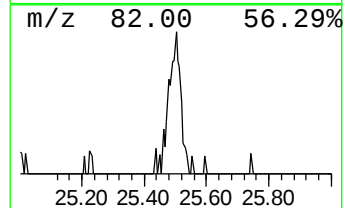
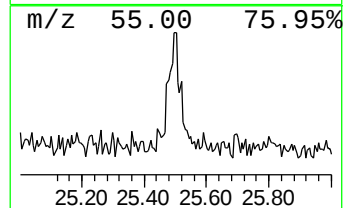
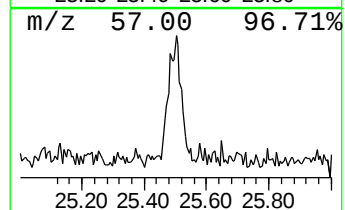
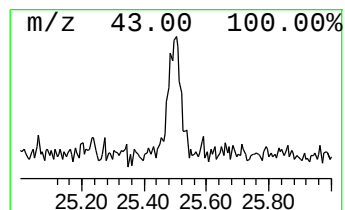
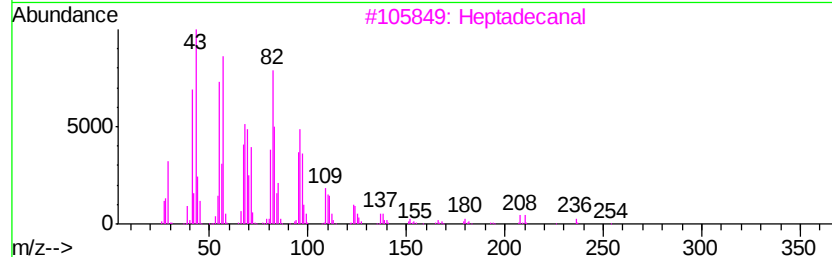
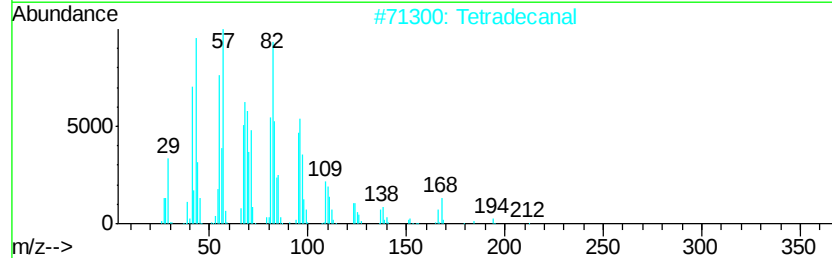
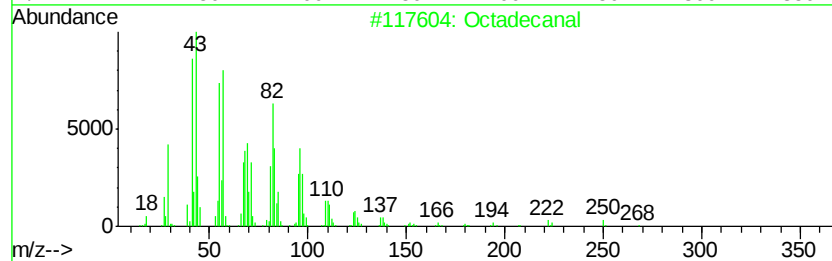
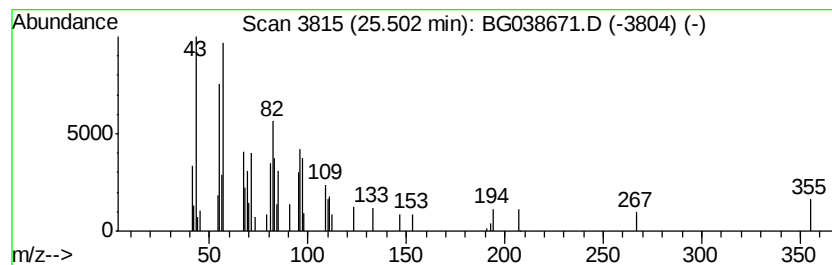
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.50	2.64 ng	51194	Perylene-d12	25.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	83
2	Tetradecanal	212	C14H28O	000124-25-4	80
3	Heptadecanal	254	C17H34O	1000376-70-0	80
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
5	9-Tetradecen-1-ol, acetate, (Z)-	254	C16H30O2	016725-53-4	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038671.D
Acq On : 17 Dec 2018 20:21
Operator : JU/SJ
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P001-SD001-0612-01

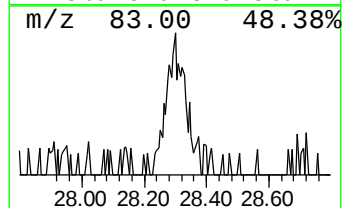
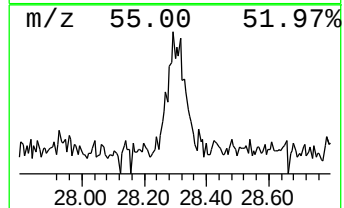
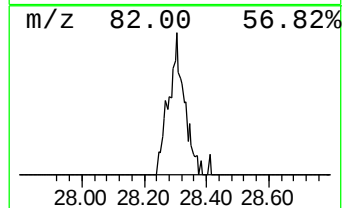
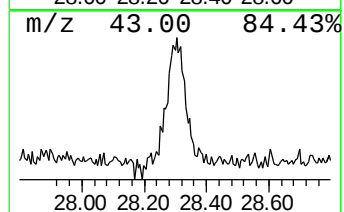
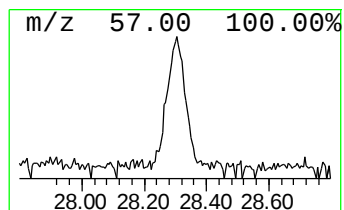
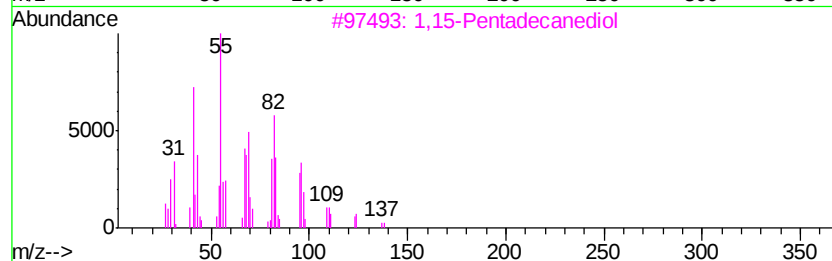
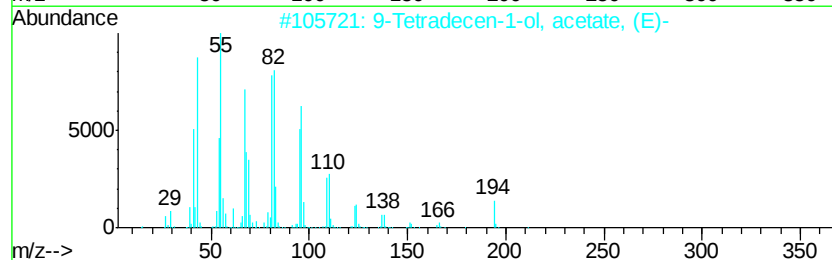
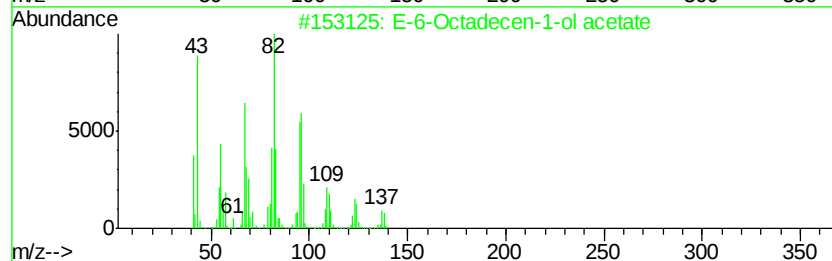
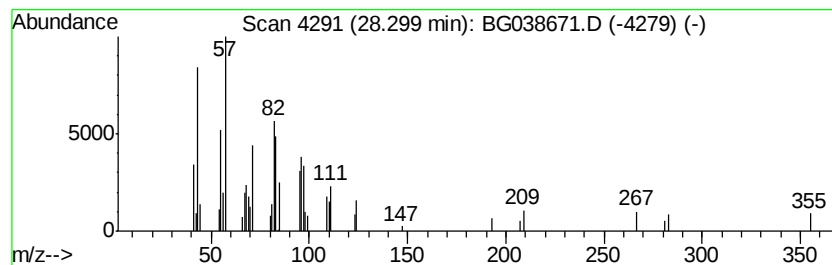
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown28.30 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.30	4.32 ng	83928	Perylene-d12	25.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-6-Octadecen-1-ol	acetate	310	C20H38O2	1000130-94-7	47	
2	9-Tetradecen-1-ol,	acetate, (E)-	254	C16H30O2	023192-82-7	47	
3	1,15-Pentadecanediol		244	C15H32O2	014722-40-8	47	
4	17-Octadecenal		266	C18H34O	056554-86-0	47	
5	Z-2-Dodecenol		184	C12H24O	069064-36-4	47	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121718\
Data File : BG038671.D
Acq On : 17 Dec 2018 20:21
Operator : JU/SJ
Sample : J6347-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P001-SD001-0612-01

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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Benzene, 1,3-dime...	6.05	13.1	ng	96359	1	8.06	147627	20.0
unknown7.59	7.59	100.0	ng	738260	1	8.06	147627	20.0
n-Hexadecanoic acid	18.30	4.0	ng	73044	4	17.44	369281	20.0
Octacosyl heptafl...	21.32	9.0	ng	183158	5	21.72	408314	20.0
Eicosane	22.48	4.5	ng	91678	5	21.72	408314	20.0
unknown22.52	22.52	3.2	ng	65084	5	21.72	408314	20.0
Eicosyl pentaflu...	23.16	2.6	ng	53366	5	21.72	408314	20.0
Heptacosane	23.99	4.2	ng	80519	6	25.02	388225	20.0
Octadecanal	25.50	2.6	ng	51194	6	25.02	388225	20.0
unknown28.30	28.30	4.3	ng	83928	6	25.02	388225	20.0