

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
 Data File : BG019851.D
 Acq On : 3 Dec 2015 1:48
 Operator : UM/NP
 Sample : G4624-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-1(10-15)

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-BG120215.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	2.996	23	27	46	rVB	902711	1250727	55.31%	10.097%
2	3.143	47	52	62	rVV3	15265	31868	1.41%	0.257%
3	5.205	397	403	410	rBV	84454	131812	5.83%	1.064%
4	5.669	475	482	491	rBV	375567	585191	25.88%	4.724%
5	7.267	746	754	768	rBV	411539	713709	31.56%	5.762%
6	7.655	812	820	828	rBV	394271	667977	29.54%	5.393%
7	8.125	894	900	907	rVB	84134	138832	6.14%	1.121%
8	8.454	949	956	964	rBV	294374	503962	22.29%	4.068%
9	9.295	1091	1099	1109	rBV	252845	446341	19.74%	3.603%
10	10.946	1373	1380	1387	rVB	119812	210814	9.32%	1.702%
11	13.384	1787	1795	1802	rBV	787672	1209644	53.50%	9.765%
12	14.206	1929	1935	1944	rBV	130532	184527	8.16%	1.490%
13	14.653	2006	2011	2016	rBV	23070	32143	1.42%	0.259%
14	14.759	2020	2029	2038	rVV2	210600	339616	15.02%	2.742%
15	15.599	2168	2172	2177	rVB	40442	49457	2.19%	0.399%
16	16.004	2231	2241	2246	rBV2	11638	29134	1.29%	0.235%
17	16.239	2274	2281	2289	rBV	664924	979714	43.33%	7.909%
18	16.463	2314	2319	2322	rBV	39091	57014	2.52%	0.460%
19	16.633	2343	2348	2353	rVV3	11869	23444	1.04%	0.189%
20	16.892	2389	2392	2400	rVB8	11249	23243	1.03%	0.188%
21	16.968	2400	2405	2408	rBV2	16782	23638	1.05%	0.191%
22	17.256	2448	2454	2457	rBV	22113	31677	1.40%	0.256%
23	17.503	2490	2496	2502	rBV	310870	452616	20.02%	3.654%
24	18.907	2730	2735	2739	rBV2	14180	22813	1.01%	0.184%
25	18.989	2745	2749	2755	rBV6	13582	23220	1.03%	0.187%
26	19.242	2788	2792	2800	rBV	27271	39129	1.73%	0.316%
27	19.788	2881	2885	2892	rVB	35235	46304	2.05%	0.374%
28	20.111	2933	2940	2945	rBV	1713601	2261140	100.00%	18.254%
29	20.317	2971	2975	2980	rBV	38964	57331	2.54%	0.463%
30	20.364	2980	2983	2989	rVV5	15297	30645	1.36%	0.247%
31	20.799	3053	3057	3064	rVB	67060	95854	4.24%	0.774%
32	20.869	3064	3069	3077	rBV7	23776	59684	2.64%	0.482%
33	21.016	3090	3094	3099	rBV	42306	70925	3.14%	0.573%
34	21.063	3099	3102	3106	rVB	77299	95720	4.23%	0.773%

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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 >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.134	3111	3114	3125	rVB2	35095	52942	2.34%	0.427%
36	21.421	3160	3163	3173	rVB4	51977	76521	3.38%	0.618%
37	21.580	3186	3190	3194	rVB2	51068	67283	2.98%	0.543%
38	21.657	3199	3203	3206	rBV4	19215	30883	1.37%	0.249%
39	21.780	3218	3224	3233	rVB	365370	625518	27.66%	5.050%
40	22.138	3282	3285	3292	rVB3	22015	35307	1.56%	0.285%
41	25.082	3778	3786	3799	rVB2	202457	578692	25.59%	4.672%

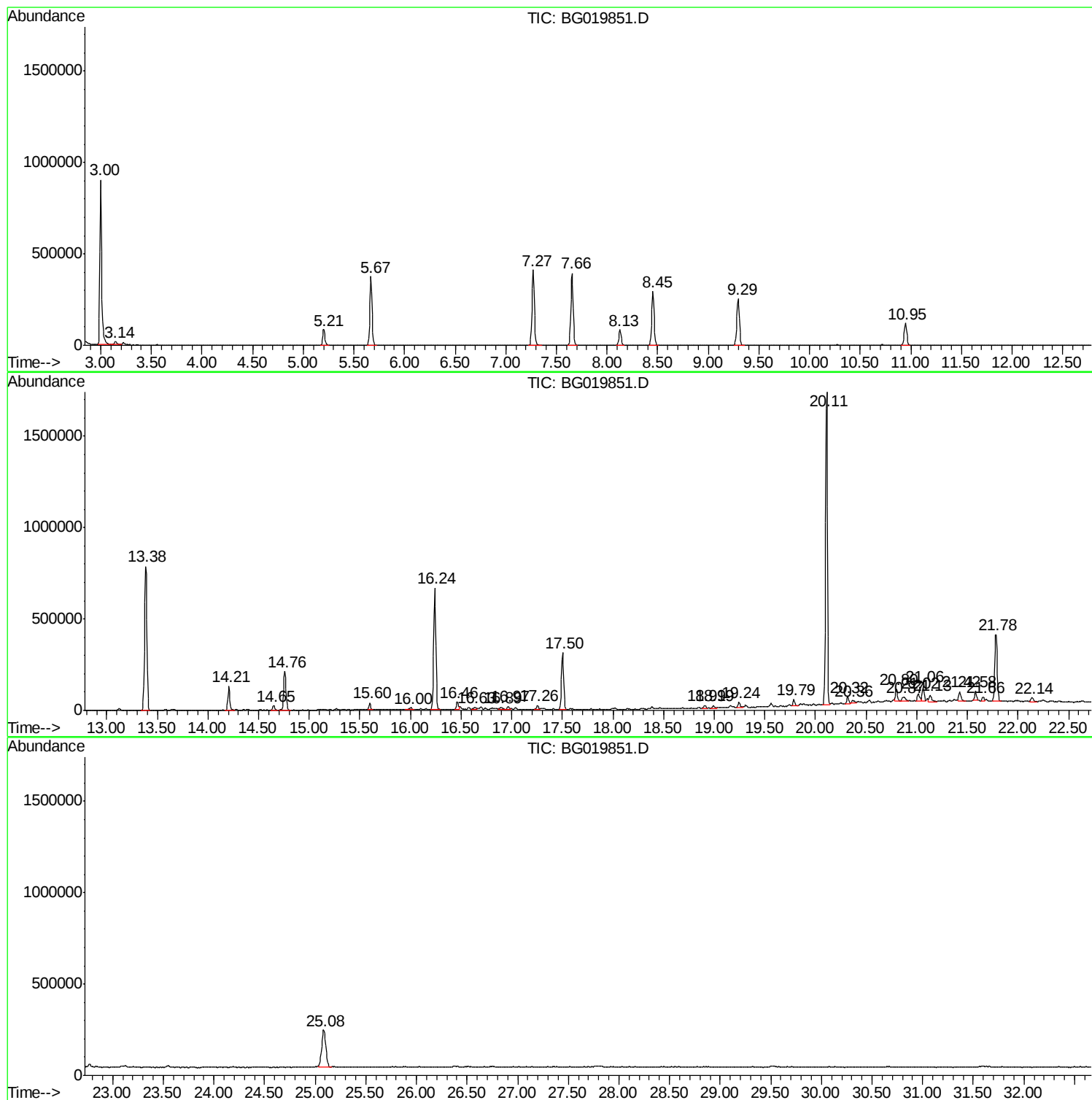
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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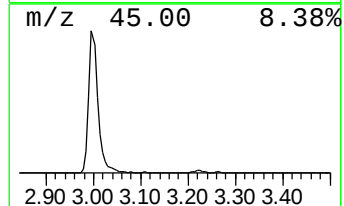
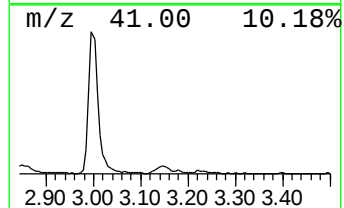
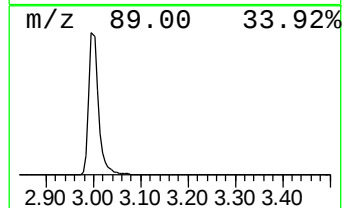
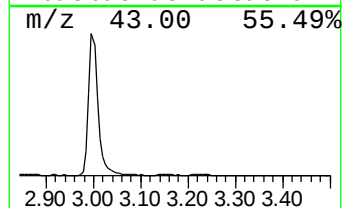
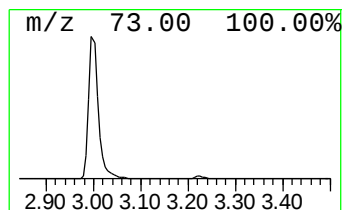
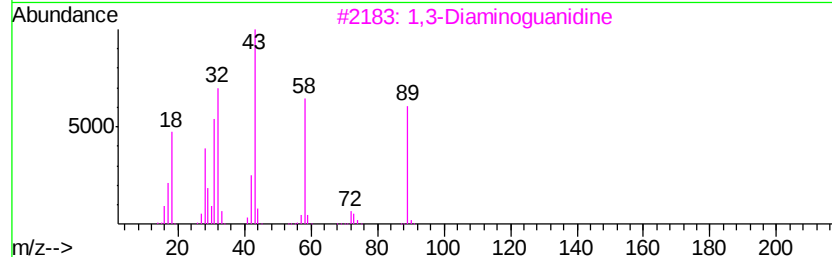
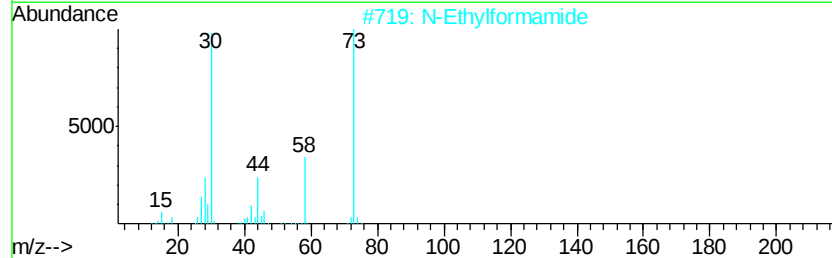
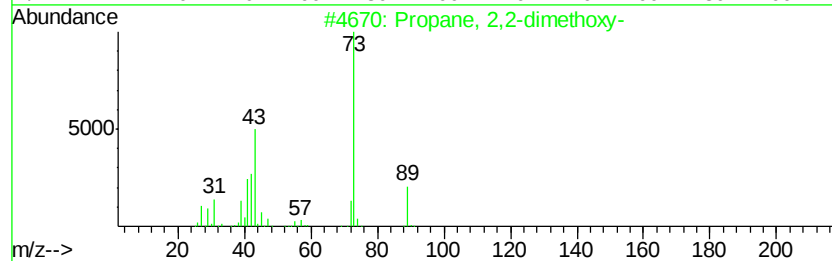
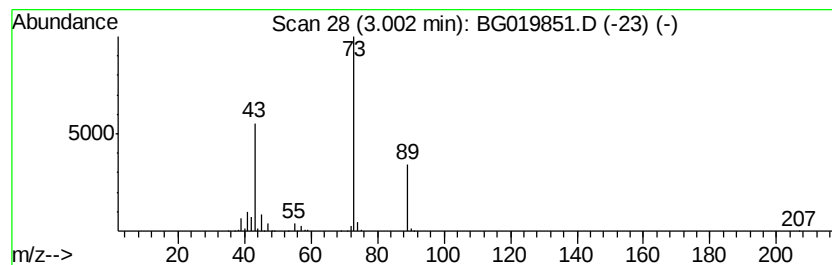
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	180.18 ng	1250730	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4		1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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Instrument :
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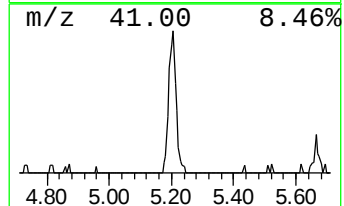
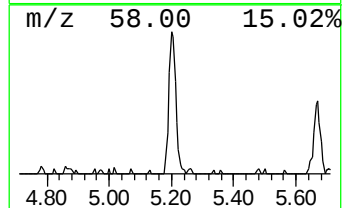
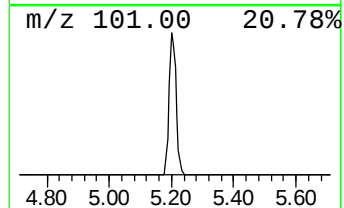
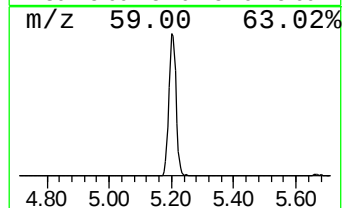
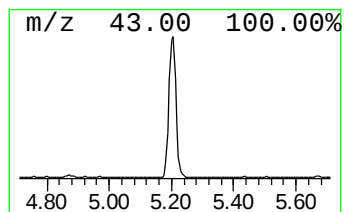
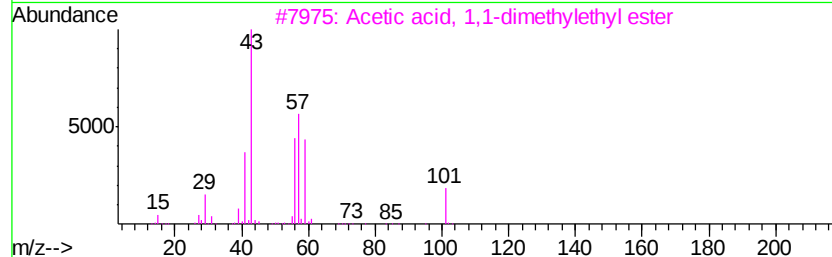
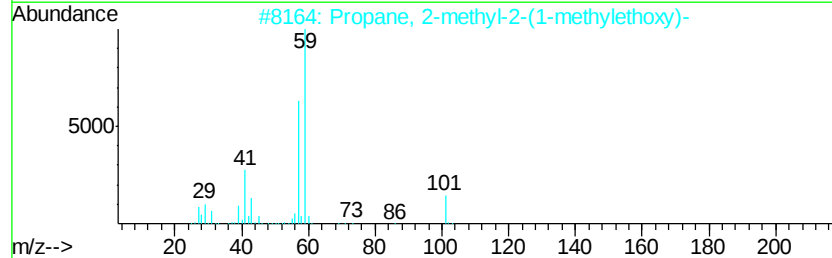
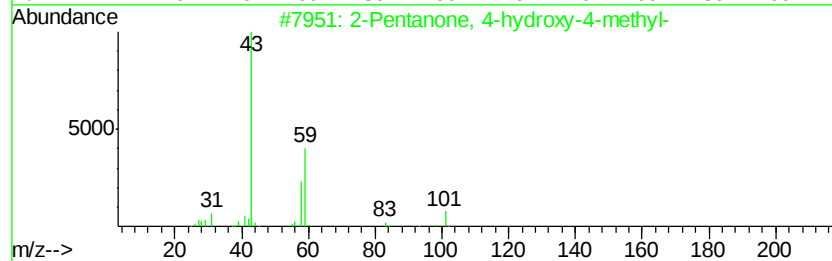
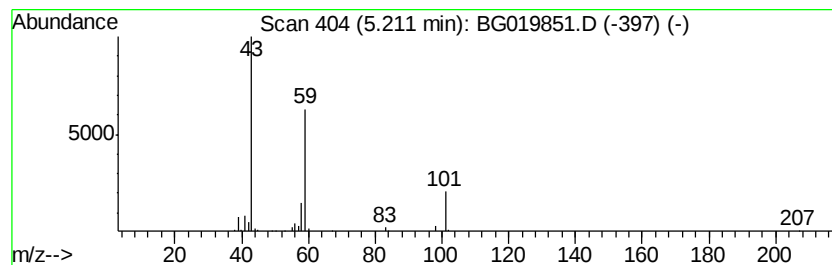
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	18.99 ng	131812	1,4-Dichlorobenzene-d4	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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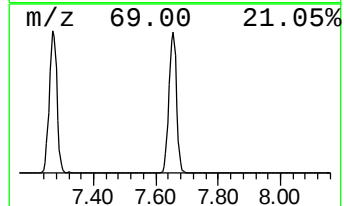
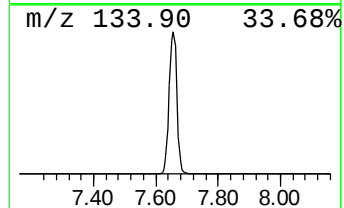
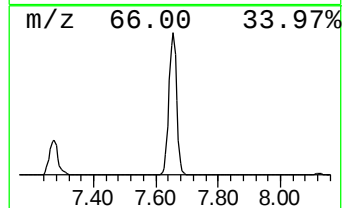
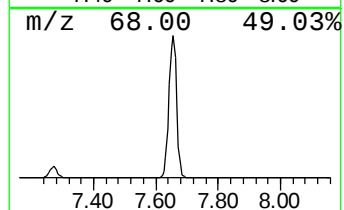
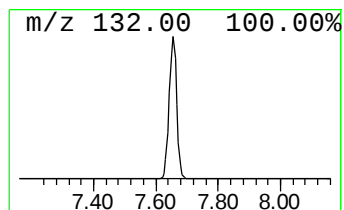
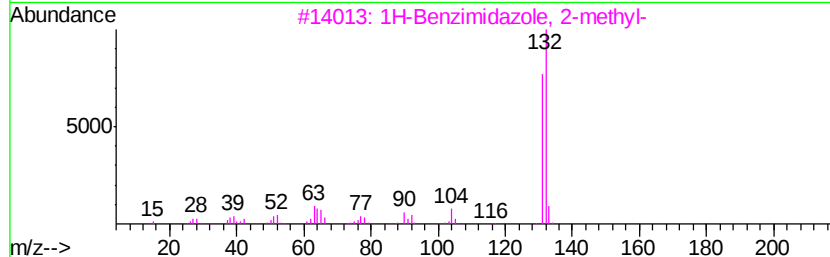
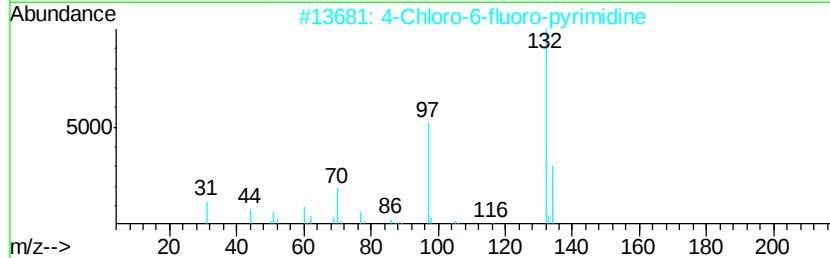
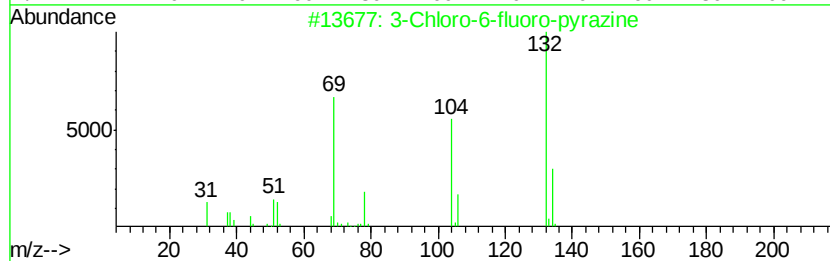
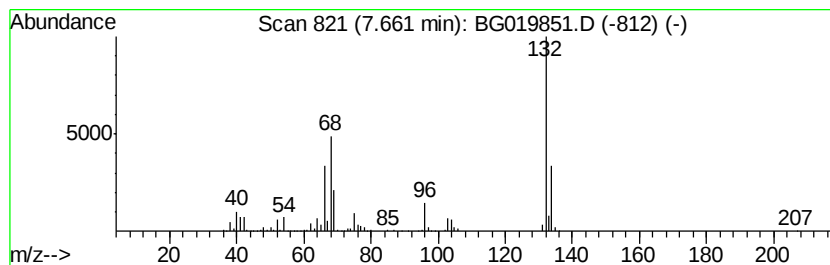
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	96.23 ng	667977	1,4-Dichlorobenzene-d4	8.13

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	10



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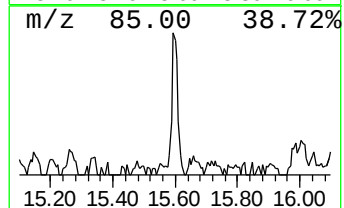
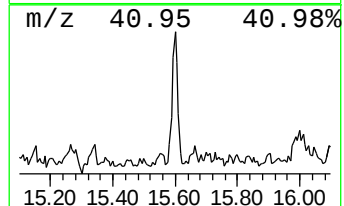
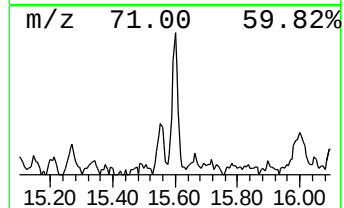
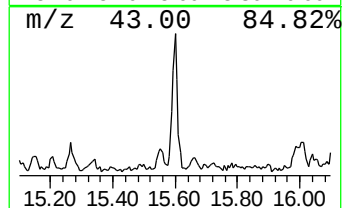
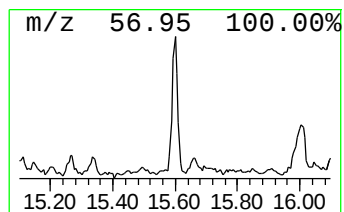
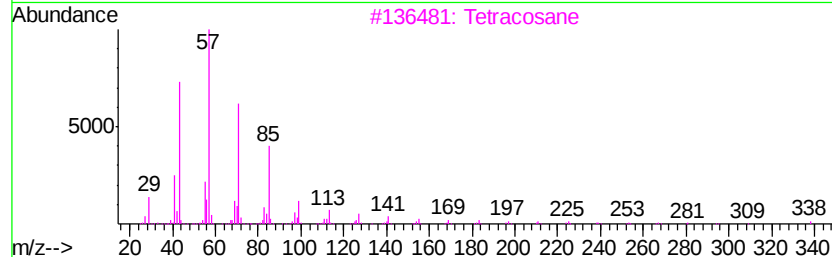
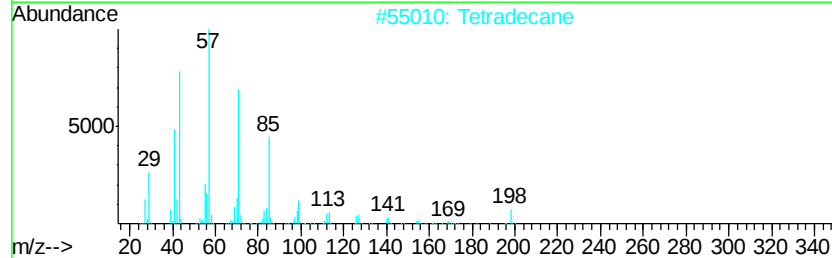
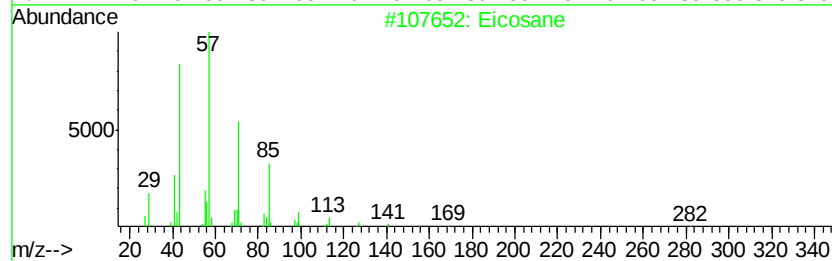
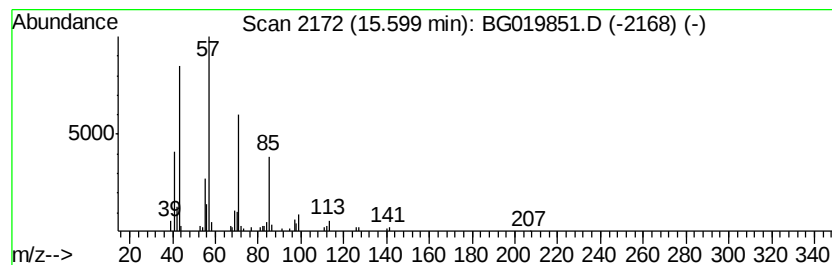
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.91 ng	49457	Acenaphthene-d10	14.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Tetradecane		198	C14H30	000629-59-4	90
3	Tetracosane		338	C24H50	000646-31-1	90
4	Octacosane		394	C28H58	000630-02-4	90
5	10-Methylnonadecane		282	C20H42	056862-62-5	90



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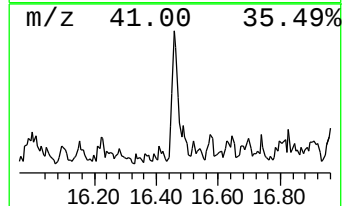
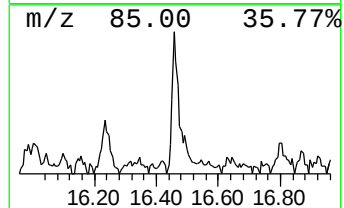
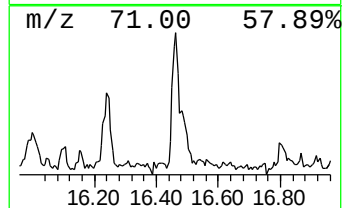
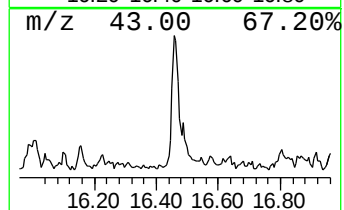
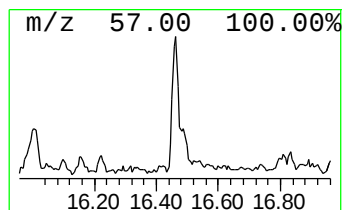
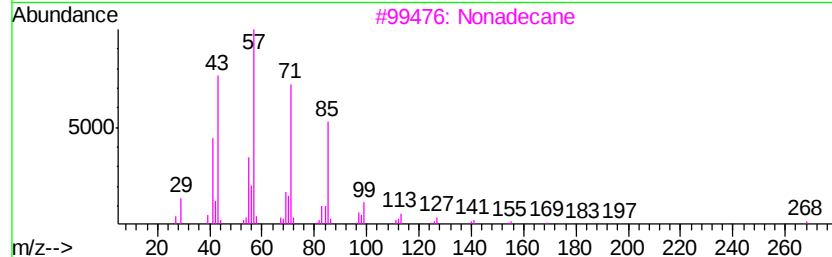
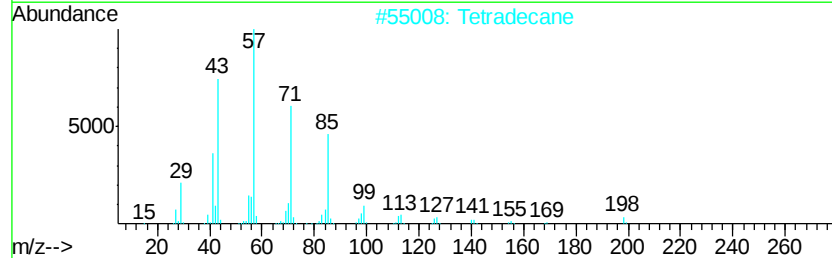
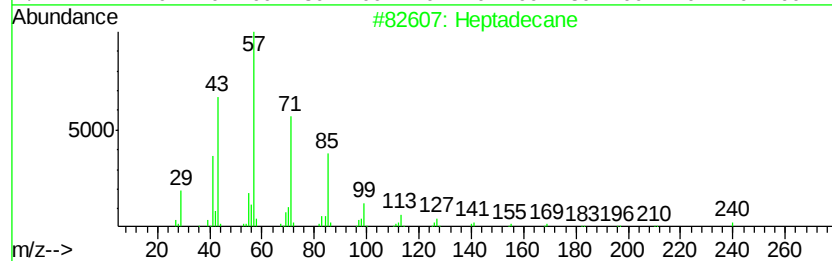
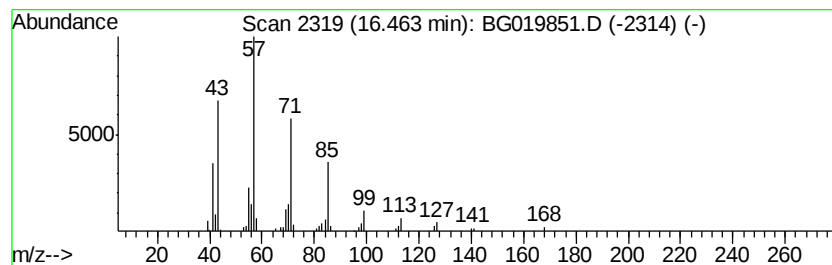
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.46	2.52 ng	57014	Phenanthrene-d10		17.50
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Tetradecane	198	C14H30	000629-59-4	91
3	Nonadecane	268	C19H40	000629-92-5	91
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	91
5	Pentadecane	212	C15H32	000629-62-9	90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
Data File : BG019851.D
Acq On : 3 Dec 2015 1:48
Operator : UM/NP
Sample : G4624-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

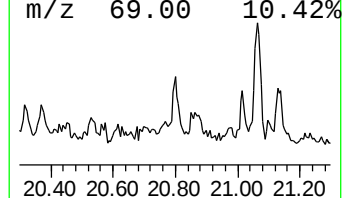
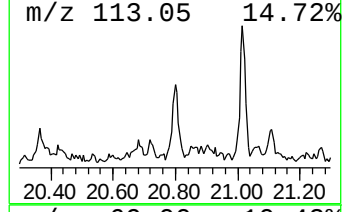
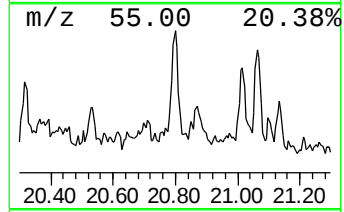
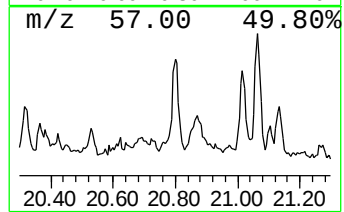
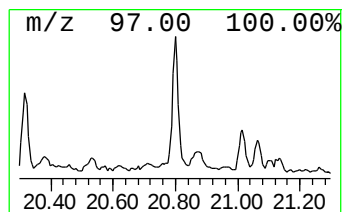
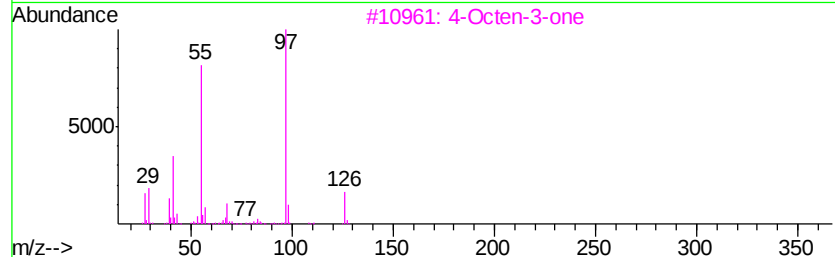
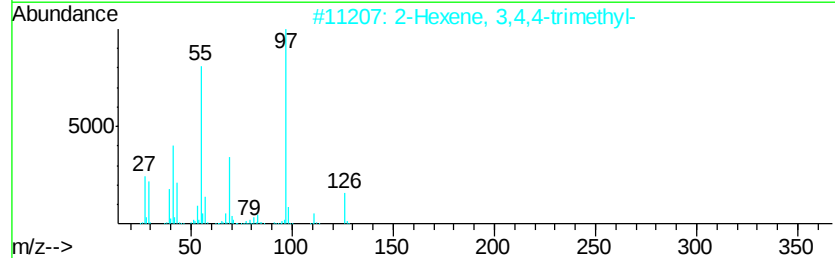
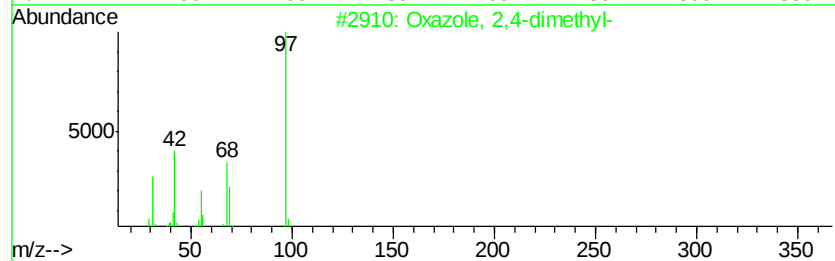
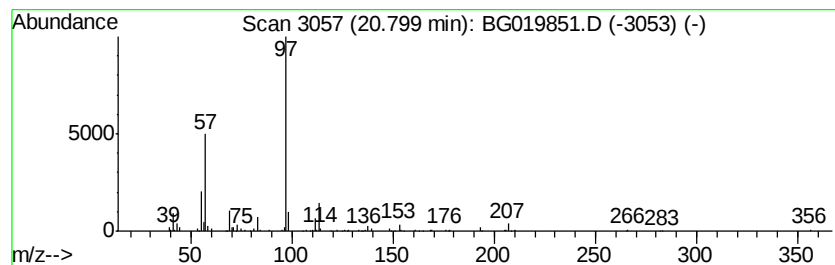
Instrument :
BNA_G
ClientSampleId :
SB-1(10-15)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Oxazole, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.80	3.06 ng	95854	Chrysene-d12	21.79	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazole, 2,4-dimethyl-	97	C5H7NO	007208-05-1	50
2	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	38
3	4-Octen-3-one	126	C8H14O	014129-48-7	36
4	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	36
5	Allyldimethyl(prop-1-ynyl)silane	138	C8H14Si	1000281-75-1	36



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
Data File : BG019851.D
Acq On : 3 Dec 2015 1:48
Operator : UM/NP
Sample : G4624-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1(10-15)

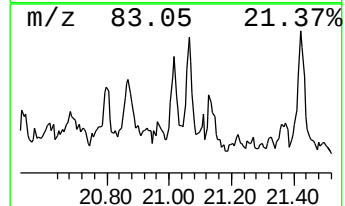
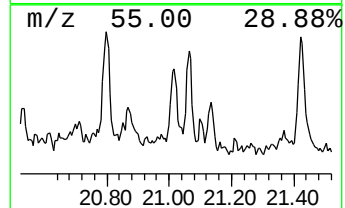
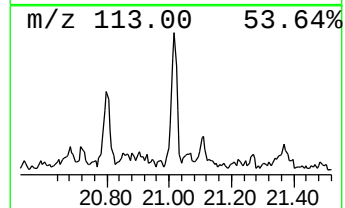
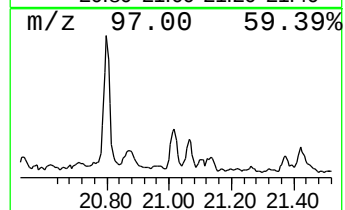
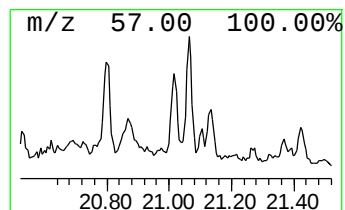
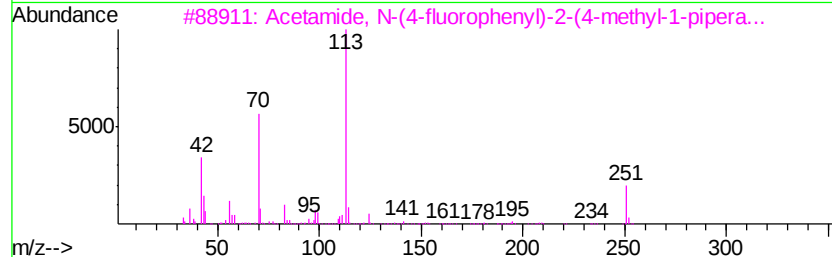
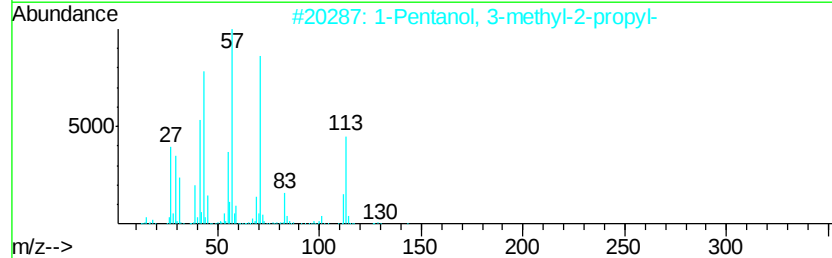
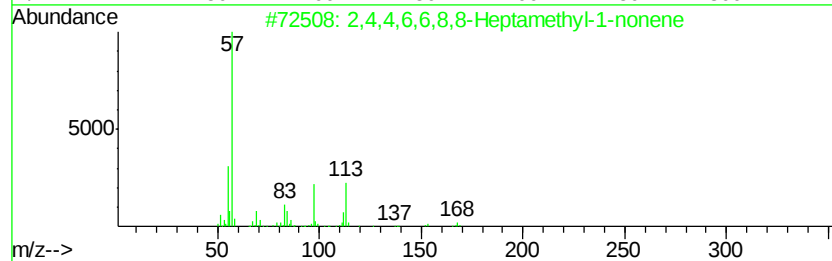
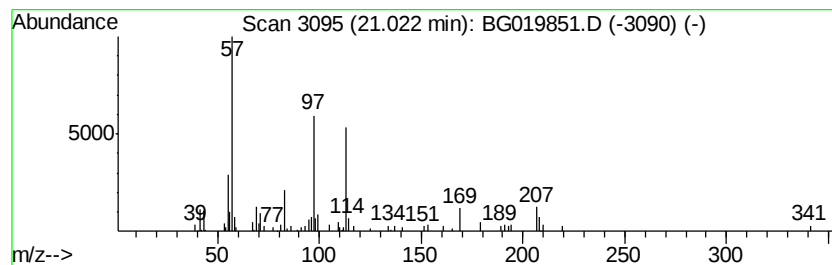
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown21.02 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.02	2.27 ng	70925	Chrysene-d12	21.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38		
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	23		
3	Acetamide, N-(4-fluorophenyl)-2-...	251	C13H18FN3O	1000267-87-7	22		
4	3-Heptene, 2,2,4,6,6-pentamethyl-	168	C12H24	000123-48-8	17		
5	Acetamide, 2-(4-methyl-1-piperaz...	267	C13H18ClN3O	296245-55-1	14		



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
Data File : BG019851.D
Acq On : 3 Dec 2015 1:48
Operator : UM/NP
Sample : G4624-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1(10-15)

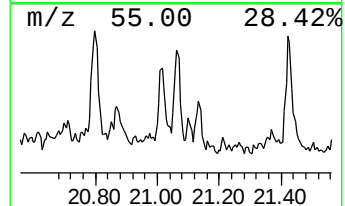
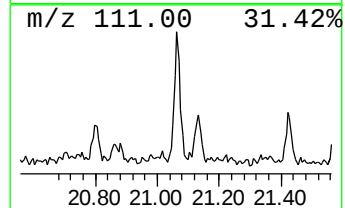
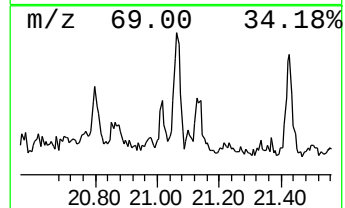
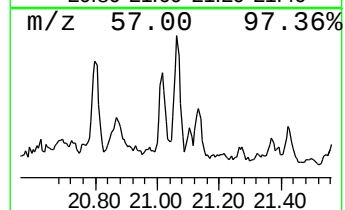
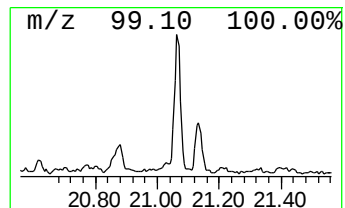
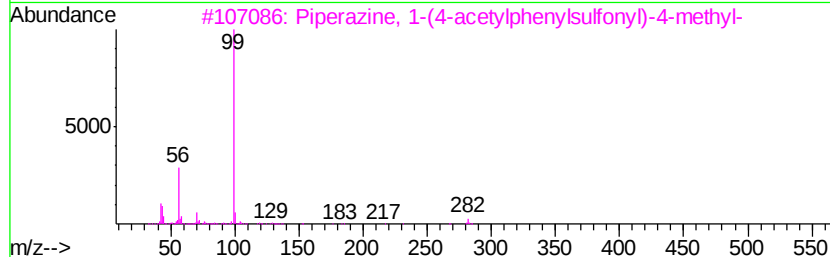
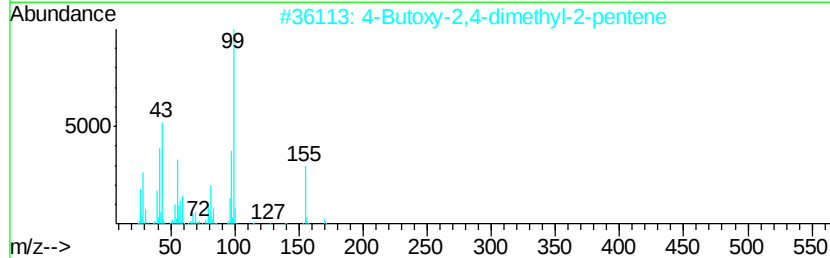
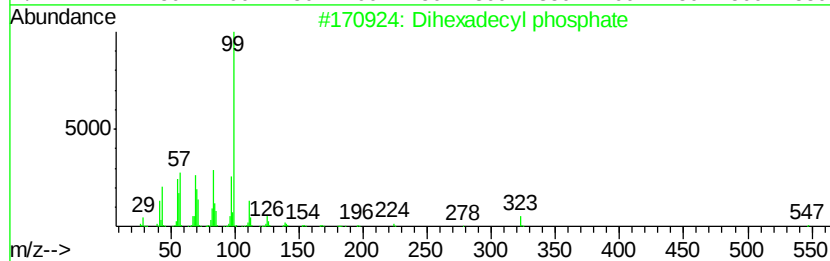
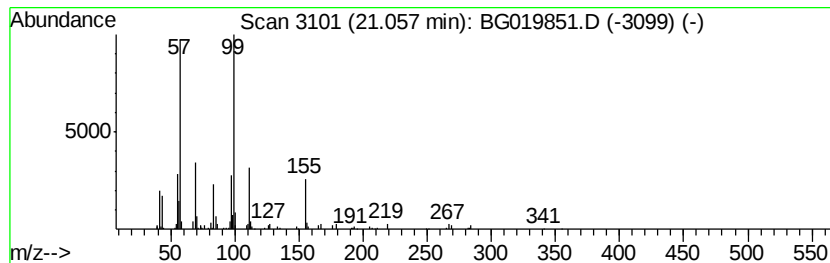
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown21.06 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	3.06 ng	95720	Chrysene-d12	21.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dihexadecyl phosphate	546	C32H67O4P	002197-63-9	42
2		4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	40
3		Piperazine, 1-(4-acetylphenylsul...	282	C13H18N2O3S	309271-25-8	35
4		Formaldehyde, dipropylhydrazone	128	C7H16N2	054253-56-4	32
5		Didodecyl phosphate	434	C24H51O4P	007057-92-3	32



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
Data File : BG019851.D
Acq On : 3 Dec 2015 1:48
Operator : UM/NP
Sample : G4624-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1(10-15)

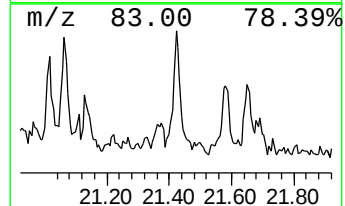
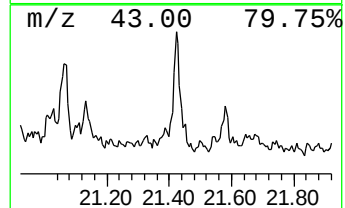
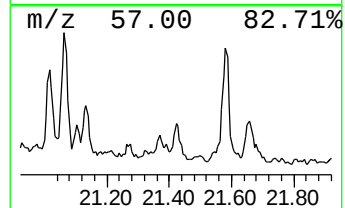
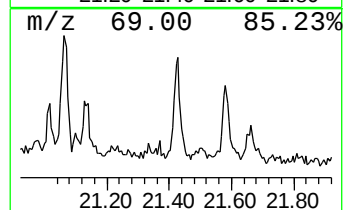
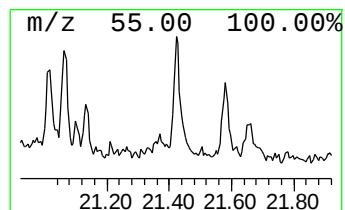
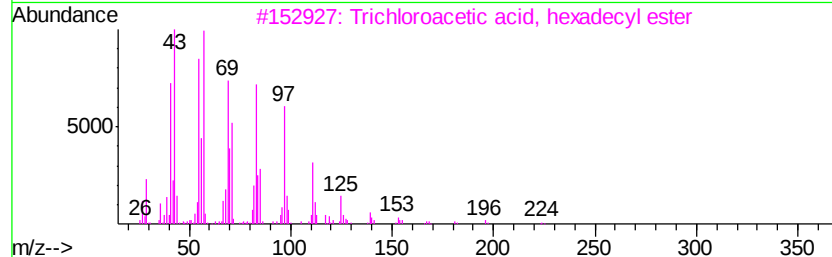
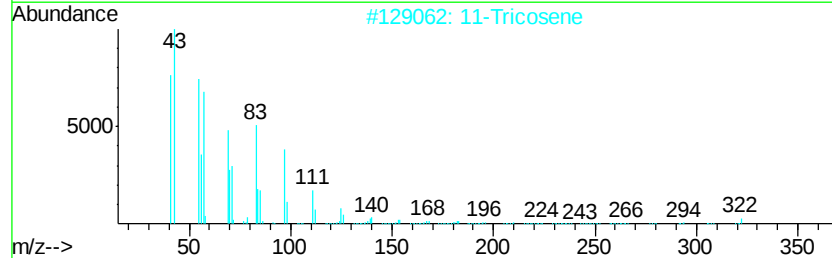
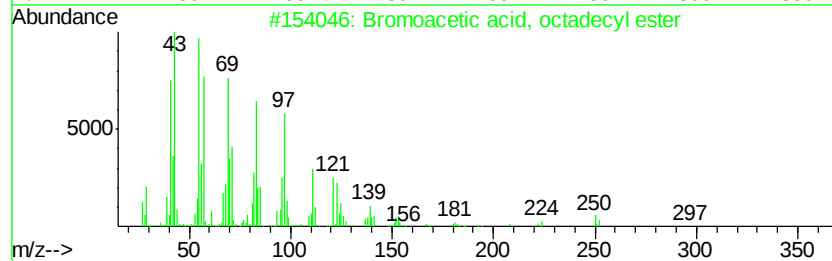
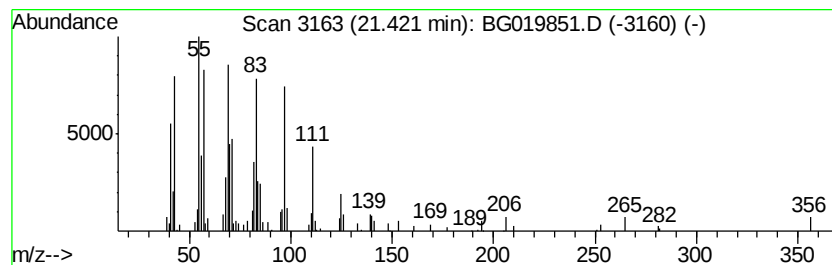
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Bromoacetic acid, octadecyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	2.45 ng	76521	Chrysene-d12	21.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2			11-Tricosene	322	C23H46	052078-56-5	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	86
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
Data File : BG019851.D
Acq On : 3 Dec 2015 1:48
Operator : UM/NP
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Instrument :
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ClientSampleId :
SB-1(10-15)

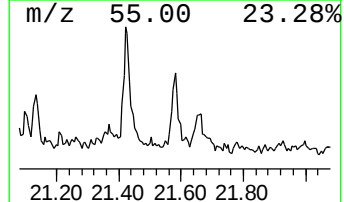
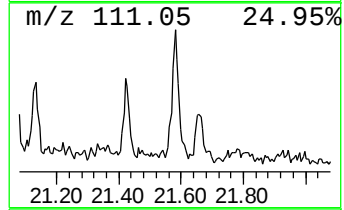
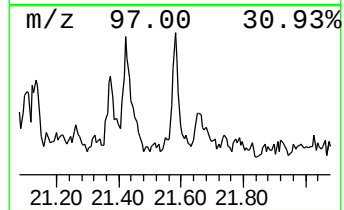
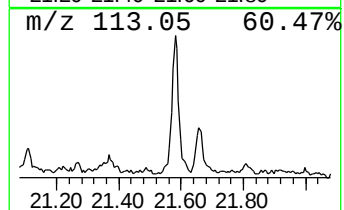
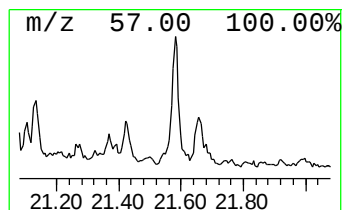
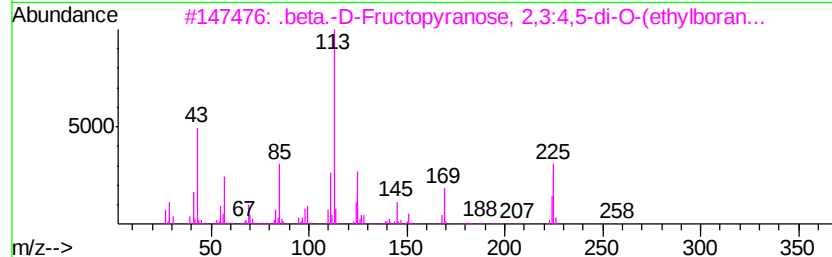
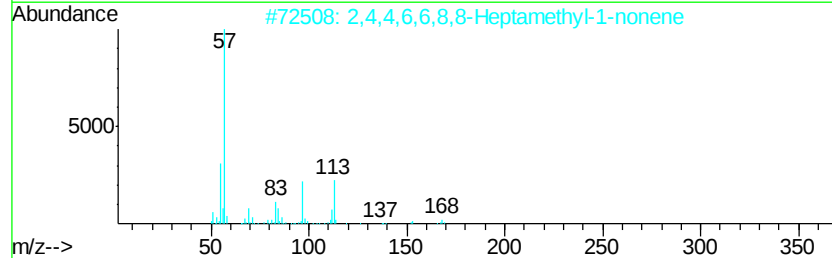
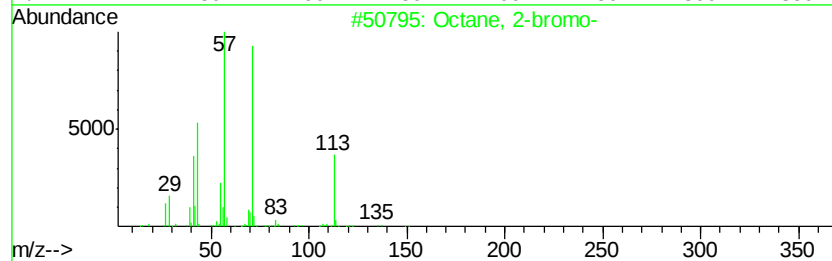
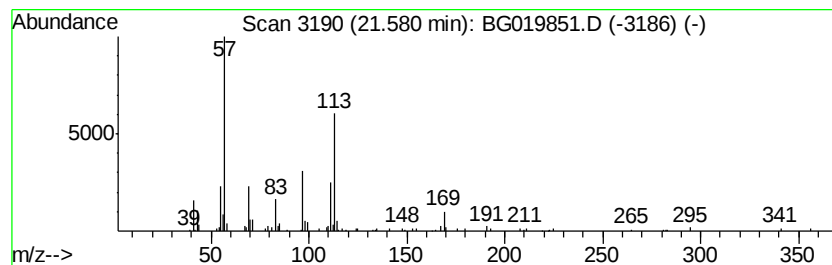
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown21.58 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.58	2.15 ng	67283	Chrysene-d12	21.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
2		2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	32
3		.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B207	1000156-76-8	32
4		N-[4-(Chloro-difluoro-methoxy)-p...	333	C14H18ClF2N3O2	1000296-77-1	22
5		Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	22



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
Data File : BG019851.D
Acq On : 3 Dec 2015 1:48
Operator : UM/NP
Sample : G4624-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-1(10-15)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.21	19.0	ng	131812	1	8.13	138832	20.0
unknown7.66	7.66	96.2	ng	667977	1	8.13	138832	20.0
Eicosane	15.60	2.9	ng	49457	3	14.76	339616	20.0
Heptadecane	16.46	2.5	ng	57014	4	17.50	452616	20.0
Oxazole, 2,4-dime...	20.80	3.1	ng	95854	5	21.79	625518	20.0
unknown21.02	21.02	2.3	ng	70925	5	21.79	625518	20.0
unknown21.06	21.06	3.1	ng	95720	5	21.79	625518	20.0
Bromoacetic acid, ...	21.42	2.5	ng	76521	5	21.79	625518	20.0
unknown21.58	21.58	2.1	ng	67283	5	21.79	625518	20.0