

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
 Data File : BG019901.D
 Acq On : 4 Dec 2015 10:54
 Operator : UM/NP
 Sample : G4609-06
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CF-3

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	22	27	44	rVV	1671600	2346207	85.01%	13.553%
2	3.137	46	51	60	rVV2	39886	81256	2.94%	0.469%
3	3.219	60	65	76	rVB	84417	121660	4.41%	0.703%
4	5.193	396	401	411	rVB	123668	188032	6.81%	1.086%
5	5.663	473	481	492	rBV	567936	890061	32.25%	5.142%
6	7.261	746	753	766	rBV	599620	1045221	37.87%	6.038%
7	7.649	810	819	826	rBV	577575	986372	35.74%	5.698%
8	8.119	893	899	905	rBV	101482	166897	6.05%	0.964%
9	8.442	947	954	964	rVB	414634	721167	26.13%	4.166%
10	9.282	1090	1097	1107	rVB	369614	658898	23.87%	3.806%
11	10.939	1372	1379	1387	rVB	150317	258871	9.38%	1.495%
12	13.378	1786	1794	1804	rVB	1055919	1648536	59.73%	9.523%
13	14.194	1927	1933	1941	rBV	314585	447658	16.22%	2.586%
14	14.747	2017	2027	2035	rBV2	252943	414235	15.01%	2.393%
15	16.233	2272	2280	2292	rBV	952315	1461619	52.96%	8.443%
16	16.445	2311	2316	2319	rBV2	21082	31993	1.16%	0.185%
17	17.490	2487	2494	2500	rBV	374802	549785	19.92%	3.176%
18	18.366	2639	2643	2650	rBV2	52258	75422	2.73%	0.436%
19	19.541	2836	2843	2849	rVB5	19308	35126	1.27%	0.203%
20	19.635	2855	2859	2864	rBV5	20670	31471	1.14%	0.182%
21	19.770	2878	2882	2888	rBV4	16020	28544	1.03%	0.165%
22	19.899	2900	2904	2908	rVB2	27205	37572	1.36%	0.217%
23	20.093	2931	2937	2943	rBV	2139904	2759860	100.00%	15.943%
24	20.299	2968	2972	2976	rBV2	20866	30335	1.10%	0.175%
25	20.781	3050	3054	3059	rVB	44659	58920	2.13%	0.340%
26	20.857	3061	3067	3074	rBV4	25938	59757	2.17%	0.345%
27	20.998	3087	3091	3095	rBV	30329	48025	1.74%	0.277%
28	21.045	3095	3099	3103	rVB	62429	77963	2.82%	0.450%
29	21.110	3108	3110	3115	rVB	25638	32742	1.19%	0.189%
30	21.398	3156	3159	3167	rVB2	40044	64765	2.35%	0.374%
31	21.556	3182	3186	3194	rVB	50462	76858	2.78%	0.444%
32	21.633	3195	3199	3208	rVB6	23123	50917	1.84%	0.294%
33	21.768	3215	3222	3230	rVB	430850	722806	26.19%	4.175%
34	23.090	3444	3447	3457	rVB5	26539	44426	1.61%	0.257%

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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

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35	23.284	3473	3480	3494	rvB	156371	329741	11.95%	1.905%
36	23.507	3513	3518	3528	rvB2	37759	81626	2.96%	0.472%
37	25.058	3771	3782	3792	rvB3	225819	645963	23.41%	3.731%

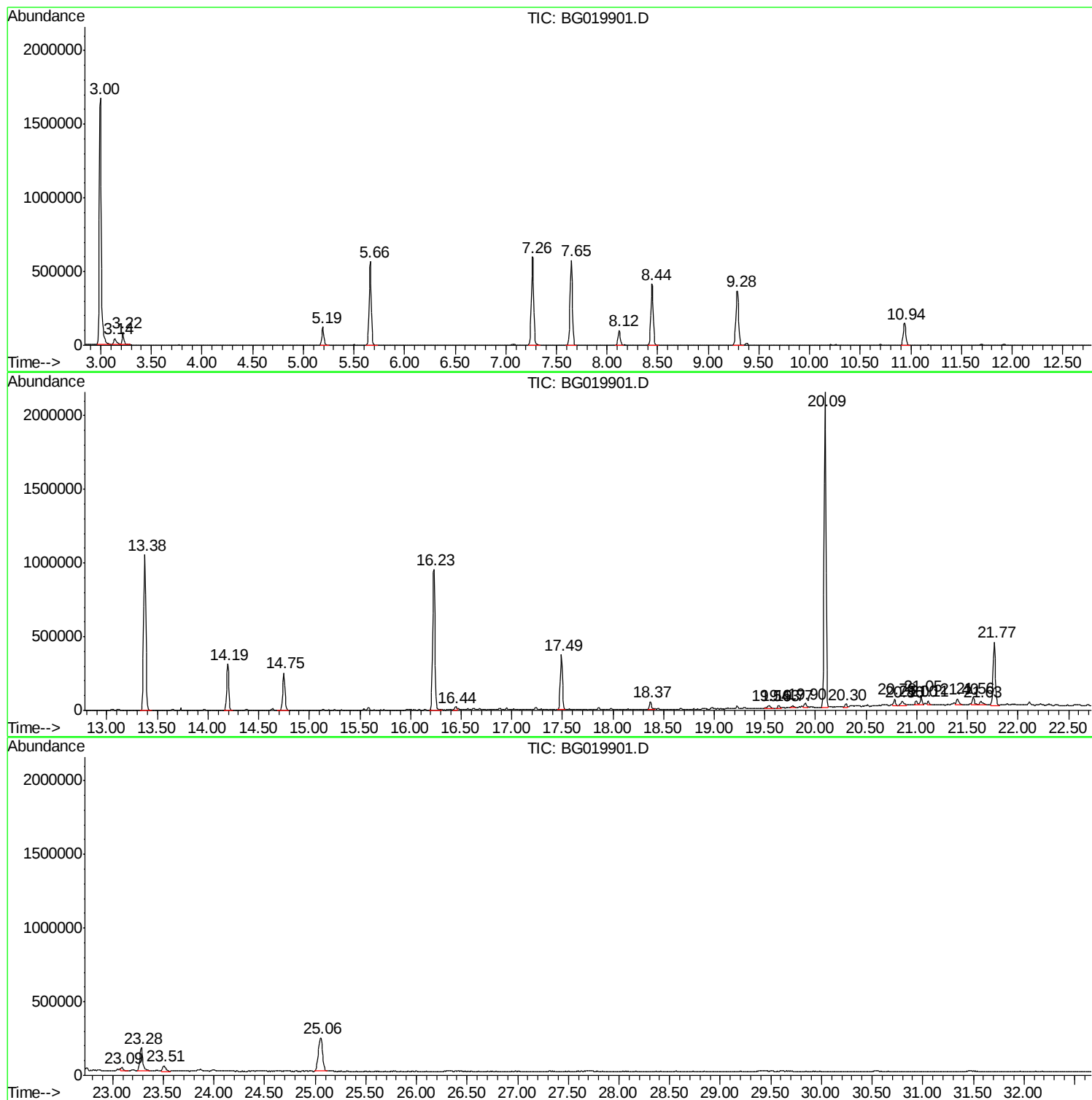
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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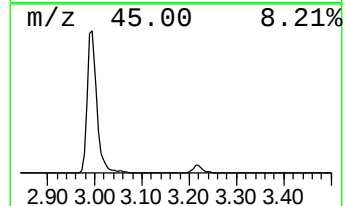
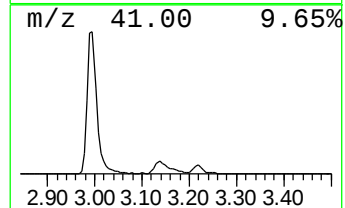
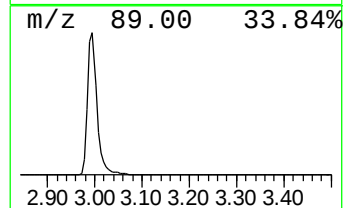
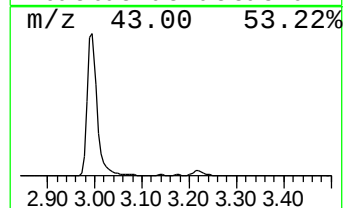
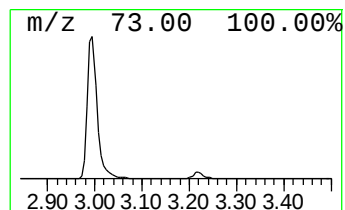
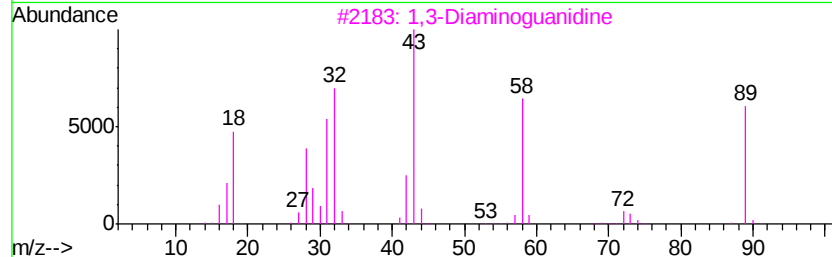
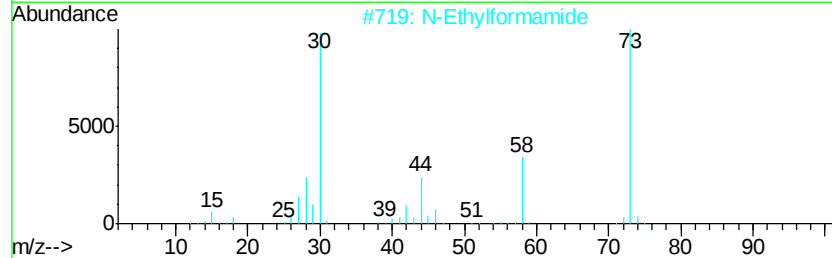
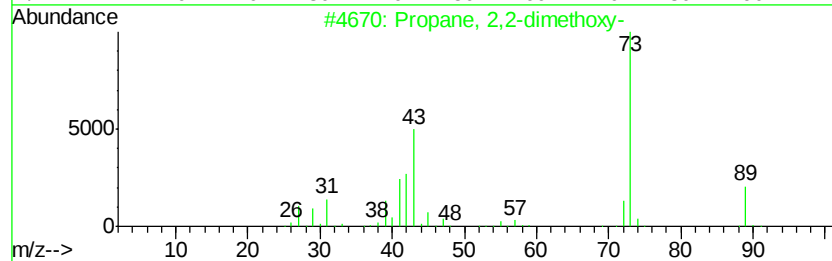
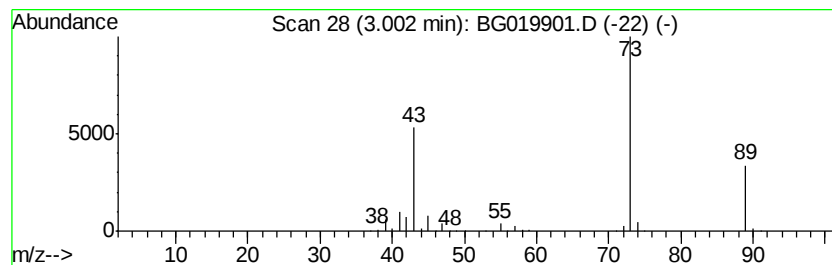
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	281.16 ng	2346210	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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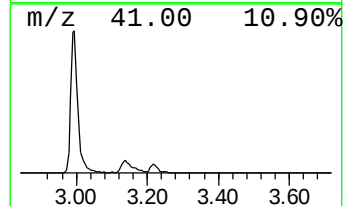
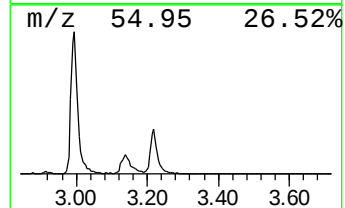
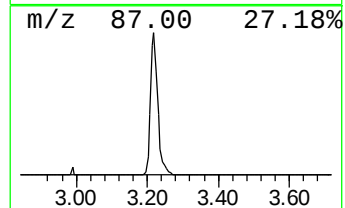
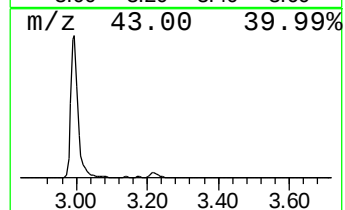
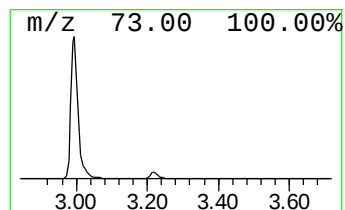
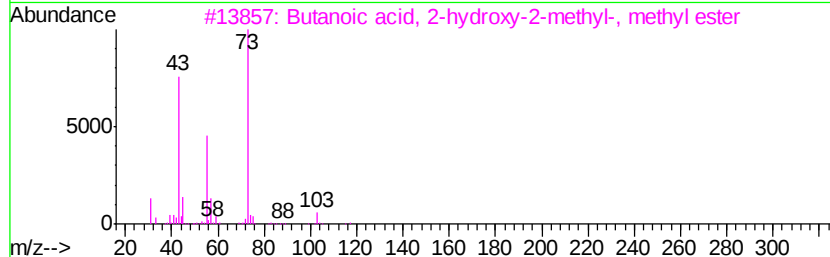
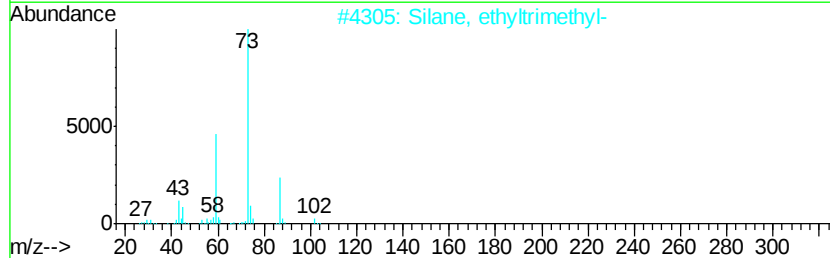
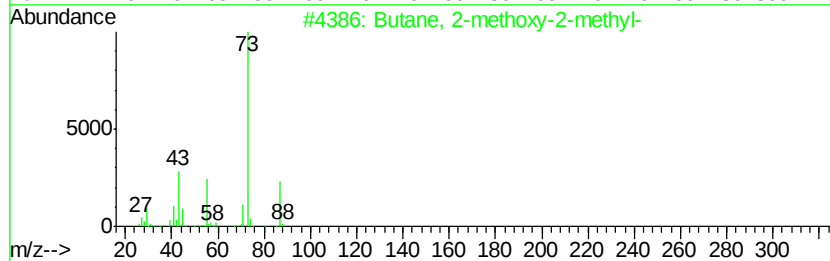
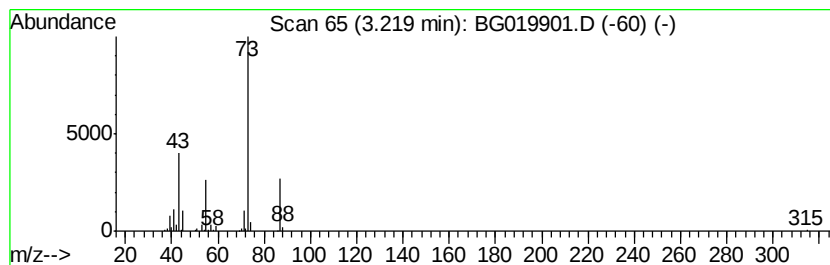
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	14.58 ng	121660	1,4-Dichlorobenzene-d4	8.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
3		Butanoic acid, 2-hydroxy-2-methyl...	132	C6H12O3	032793-34-3	12
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Disilane, ethylpentamethyl-	160	C7H20Si2	015063-64-6	9



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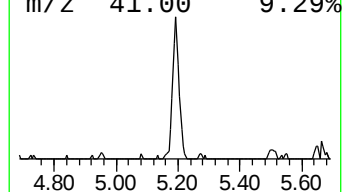
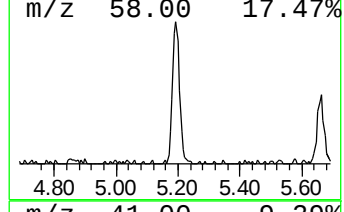
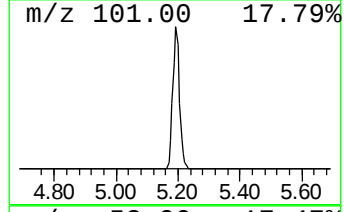
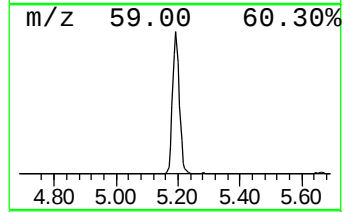
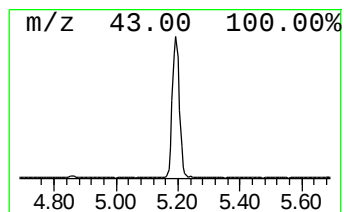
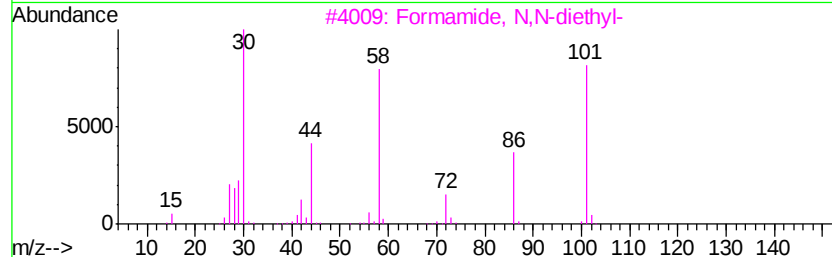
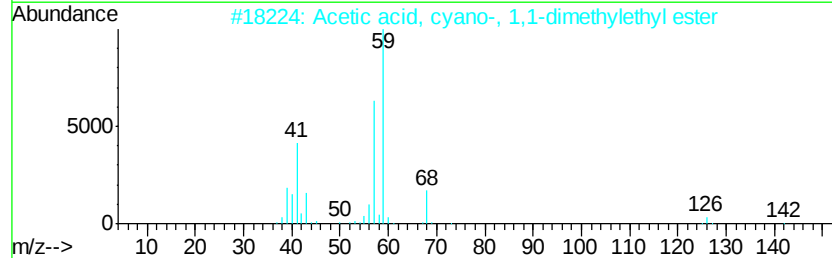
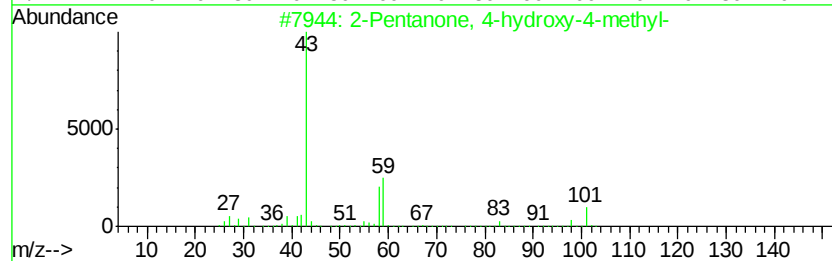
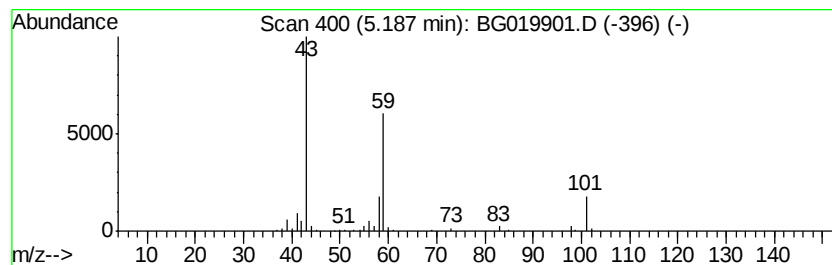
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	22.53 ng	188032	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane	58	C4H10	000106-97-8	9



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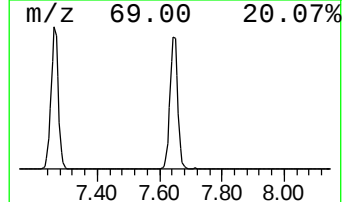
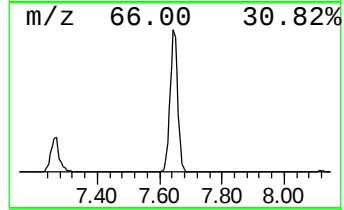
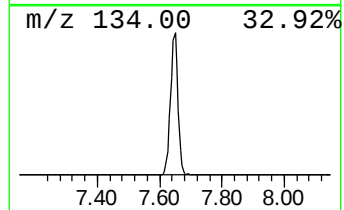
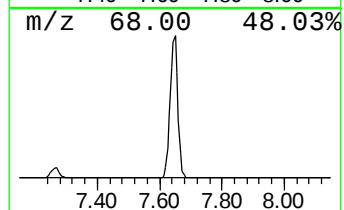
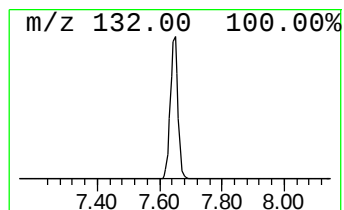
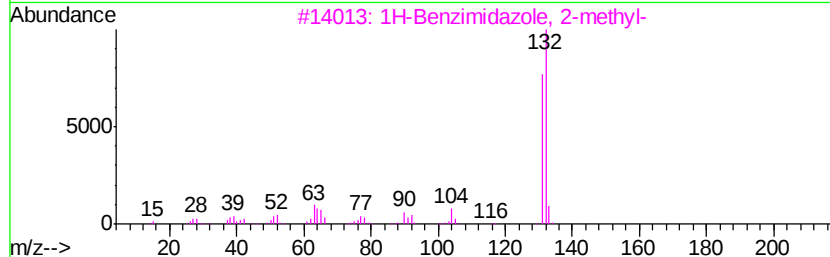
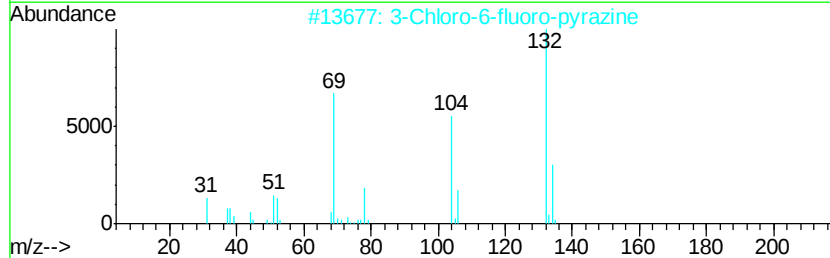
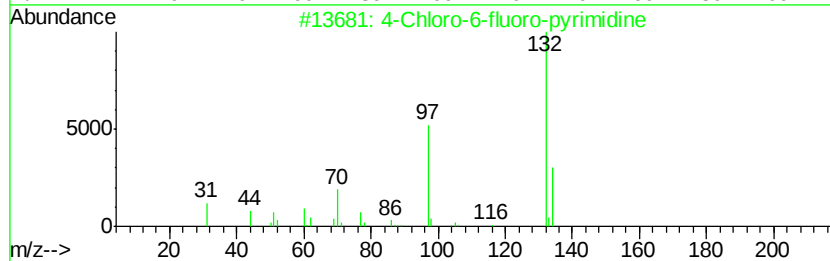
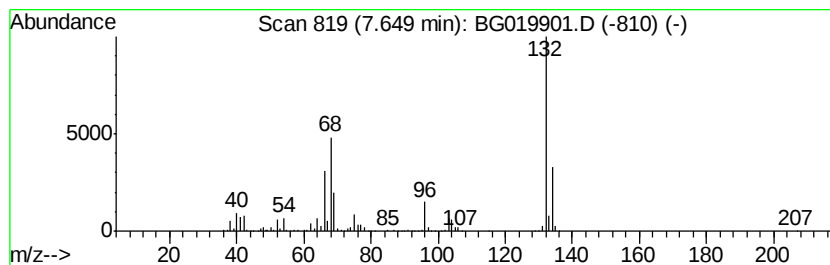
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	118.20 ng	986372	1,4-Dichlorobenzene-d4	8.12

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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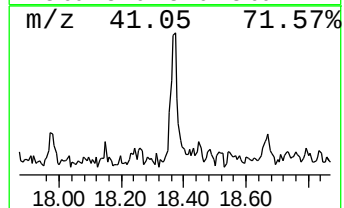
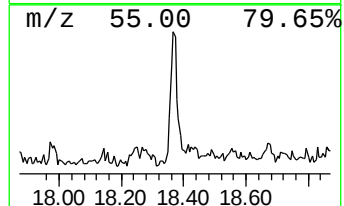
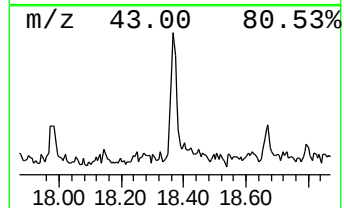
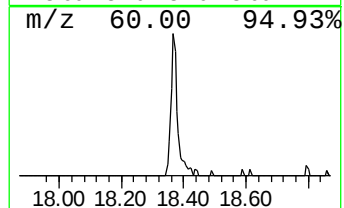
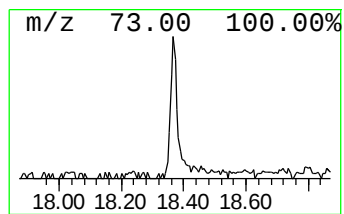
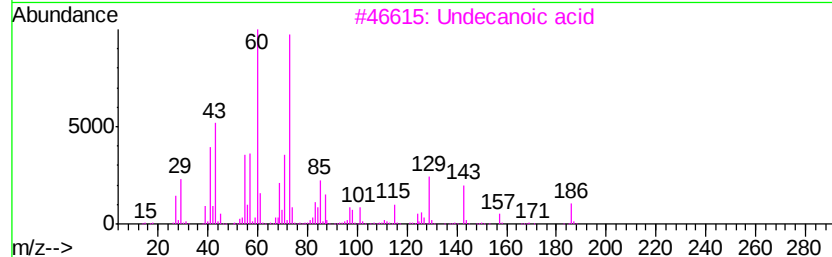
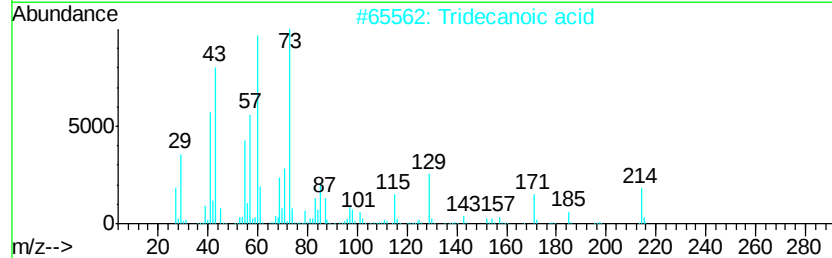
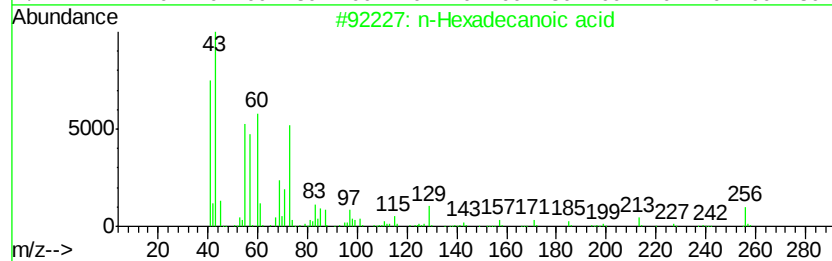
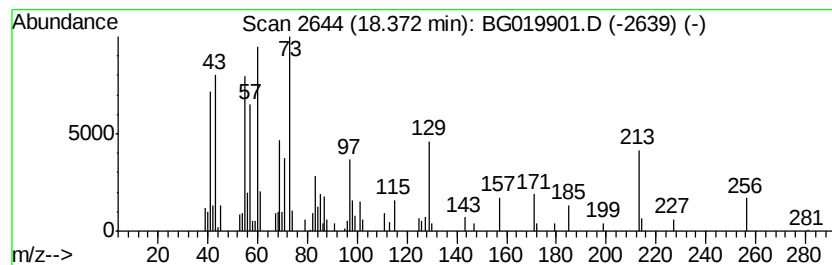
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	2.74 ng	75422	Phenanthrene-d10	17.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Undecanoic acid	186	C11H22O2	000112-37-8	59
4		Dodecanoic acid	200	C12H24O2	000143-07-7	59
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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Sample : G4609-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CF-3

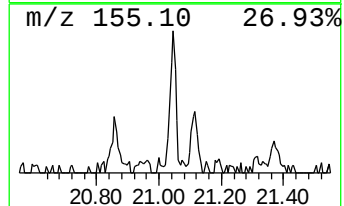
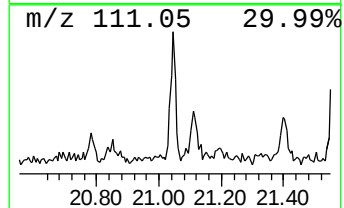
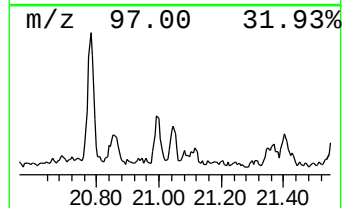
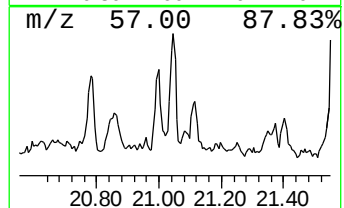
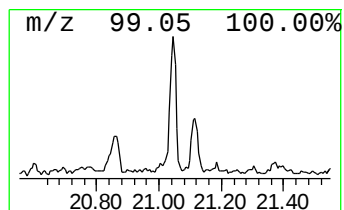
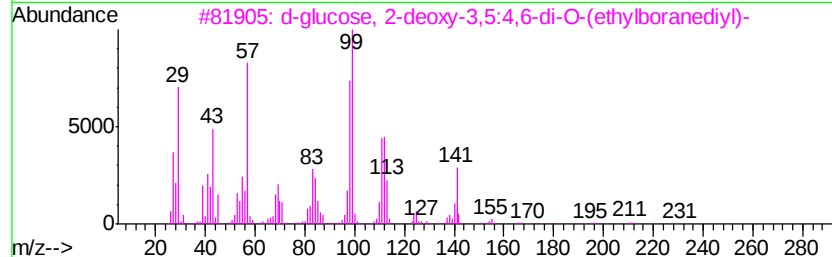
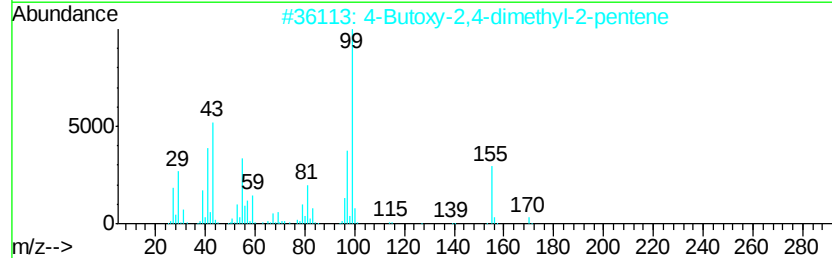
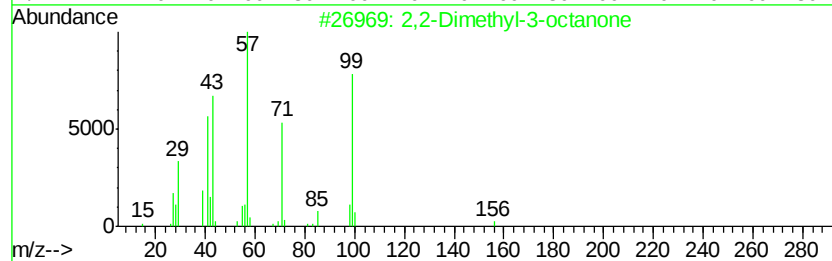
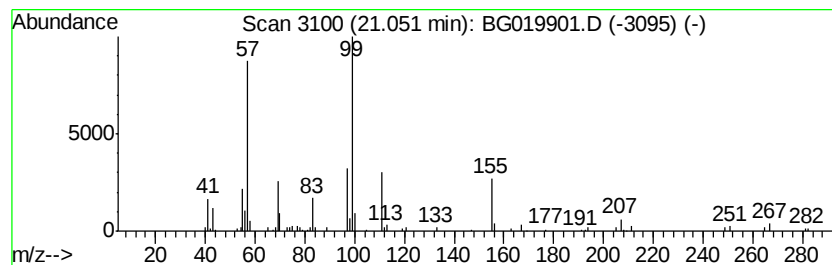
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown21.05 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.05	2.16 ng	77963	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	43
2		4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	42
3		d-glucose, 2-deoxy-3,5:4,6-di-O-...	240	C10H18B2O5	1000149-94-7	36
4		2-Propylthiazole	127	C6H9NS	017626-75-4	27
5		Spiro[bicyclo[2.2.1]heptane-2,2'...	210	C12H18O3	018501-54-7	27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019901.D
Acq On : 4 Dec 2015 10:54
Operator : UM/NP
Sample : G4609-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CF-3

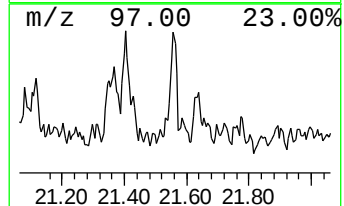
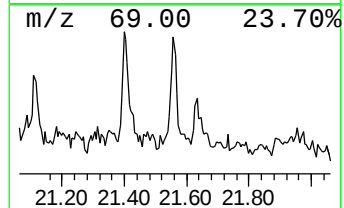
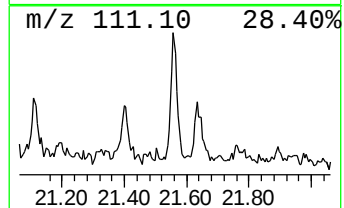
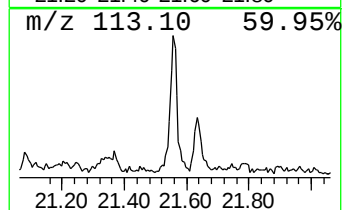
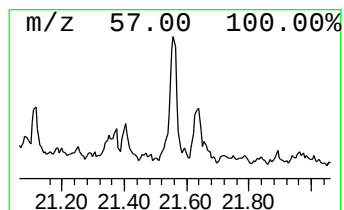
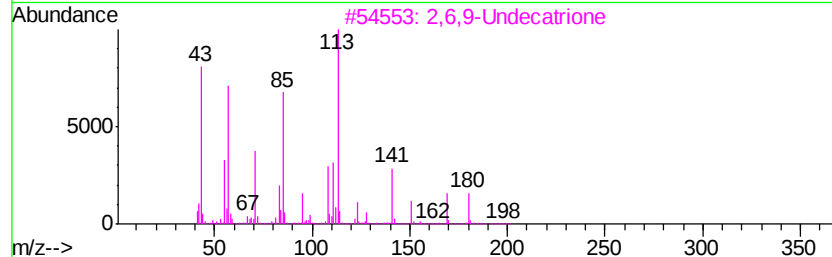
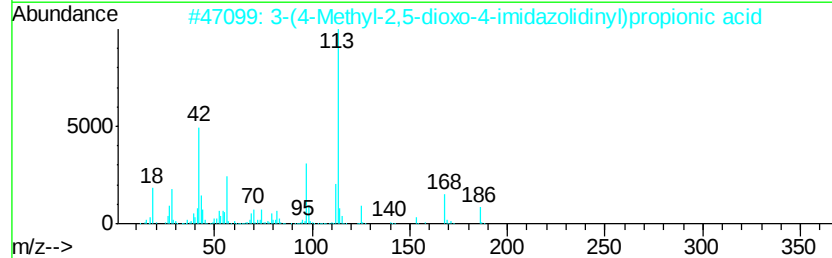
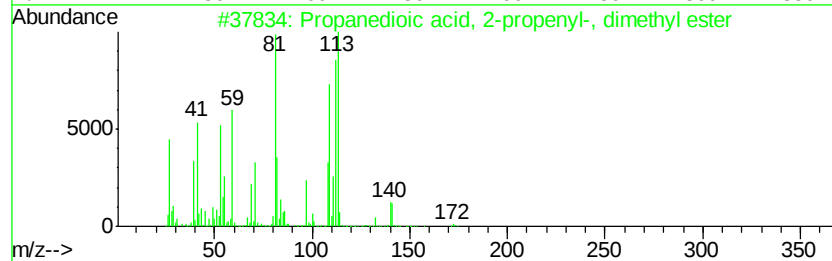
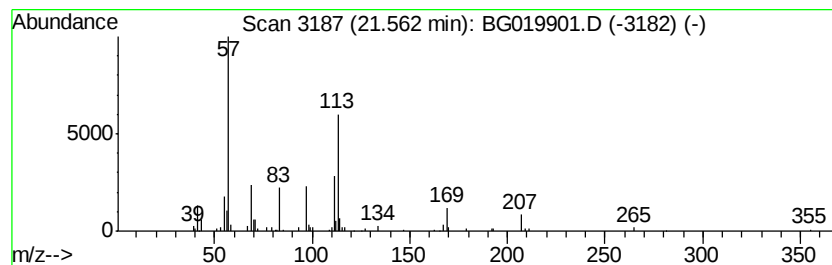
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown21.56 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.56	2.13 ng	76858	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	25
2		3-(4-Methyl-2,5-dioxo-4-imidazol...	186	C7H10N2O4	007511-46-8	25
3		2,6,9-Undecatriene	198	C11H18O3	078975-91-4	23
4		1-Ethyl-2,2-dimethylpropyl ethyl...	210	C9H20F02P	1000298-32-8	17
5		4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	14



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019901.D
Acq On : 4 Dec 2015 10:54
Operator : UM/NP
Sample : G4609-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CF-3

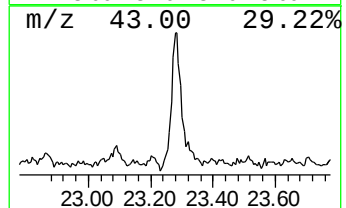
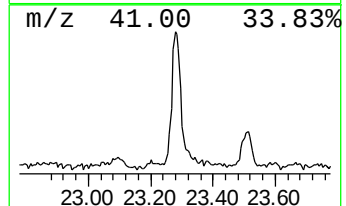
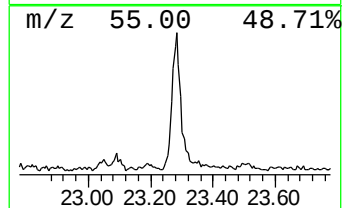
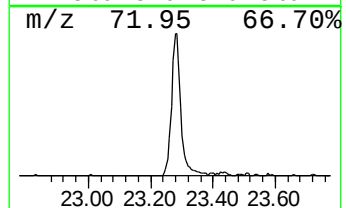
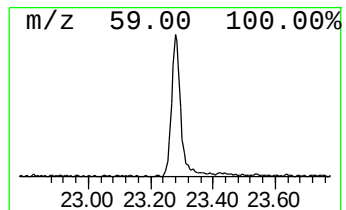
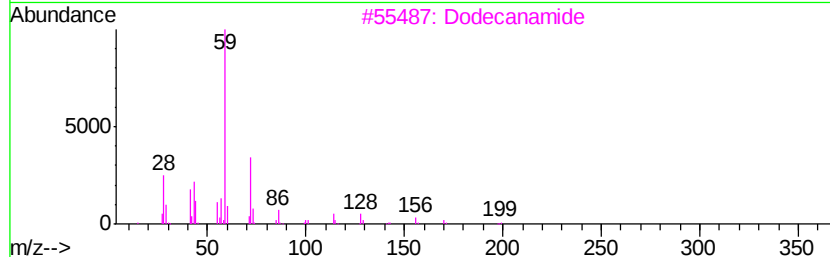
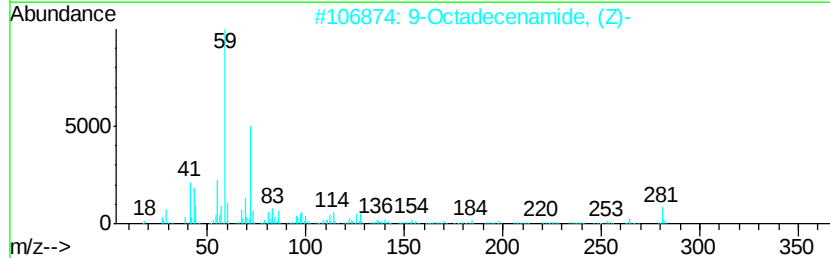
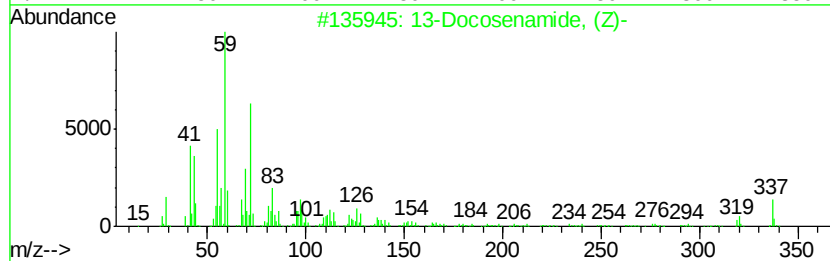
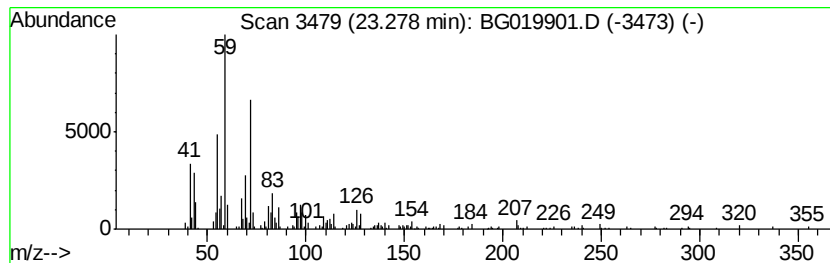
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	9.12 ng	329741	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
3		Dodecanamide	199	C12H25NO	001120-16-7	53
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53
5		Hexadecanamide	255	C16H33NO	000629-54-9	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019901.D
Acq On : 4 Dec 2015 10:54
Operator : UM/NP
Sample : G4609-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CF-3

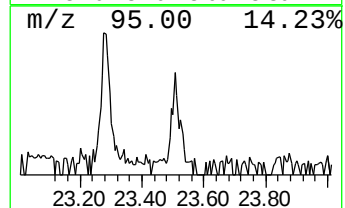
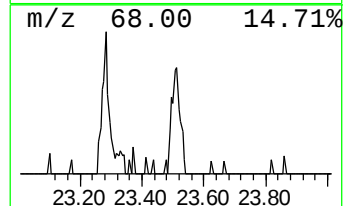
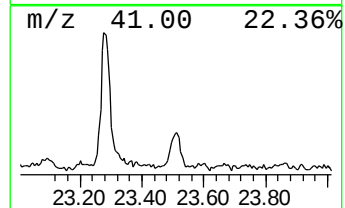
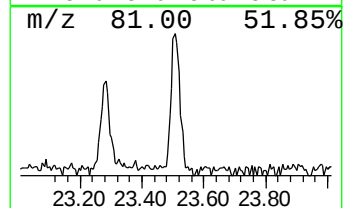
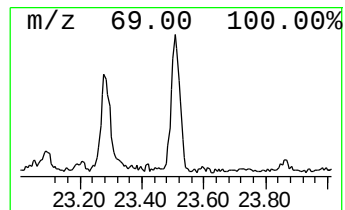
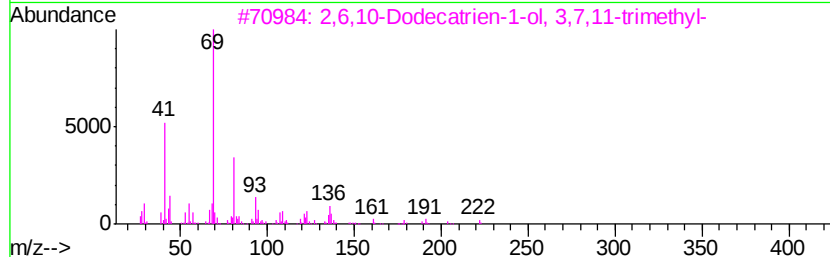
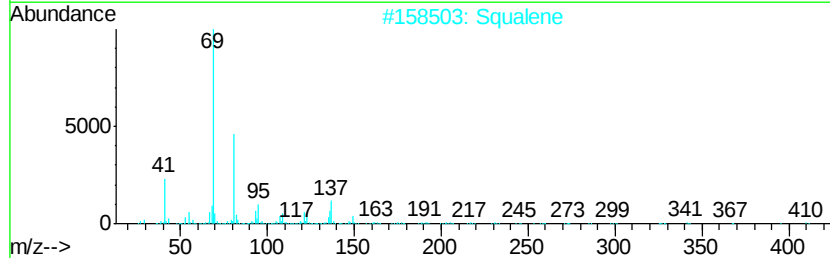
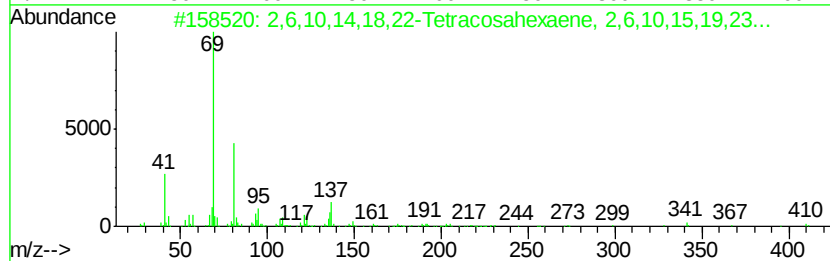
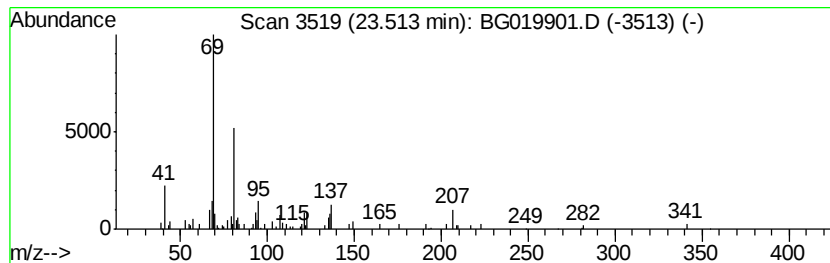
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.51	2.53 ng	81626	Perylene-d12	25.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87		
2	Squalene	410	C30H50	007683-64-9	80		
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	76		
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	64		
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	56		



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120315\
Data File : BG019901.D
Acq On : 4 Dec 2015 10:54
Operator : UM/NP
Sample : G4609-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	3.00	281.2	ng	2346210	1	8.12	166897	20.0
Butane, 2-methoxy...	3.22	14.6	ng	121660	1	8.12	166897	20.0
2-Pentanone, 4-hy...	5.19	22.5	ng	188032	1	8.12	166897	20.0
unknown7.65	7.65	118.2	ng	986372	1	8.12	166897	20.0
n-Hexadecanoic acid	18.37	2.7	ng	75422	4	17.49	549785	20.0
unknown21.05	21.05	2.2	ng	77963	5	21.77	722806	20.0
unknown21.56	21.56	2.1	ng	76858	5	21.77	722806	20.0
13-Docosenamide, ...	23.28	9.1	ng	329741	5	21.77	722806	20.0
2,6,10,14,18,22-T...	23.51	2.5	ng	81626	6	25.05	645963	20.0