

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
 Data File : BG018643.D
 Acq On : 11 Sep 2015 17:30
 Operator : UM/IZ
 Sample : G3612-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-21

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-BG091115.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	2.891	5	9	16	rVB	35988	43080	1.12%	0.166%
2	2.962	16	21	40	rVB	2853011	3852384	100.00%	14.874%
3	3.109	40	46	53	rBV2	46974	82790	2.15%	0.320%
4	3.179	53	58	72	rVB	662453	919350	23.86%	3.550%
5	5.106	380	386	393	rBV	376776	553411	14.37%	2.137%
6	5.576	459	466	478	rBV	845658	1294786	33.61%	4.999%
7	7.169	727	737	750	rBV	870894	1442306	37.44%	5.569%
8	7.539	793	800	809	rBV	835143	1411328	36.64%	5.449%
9	8.003	873	879	886	rBV	192863	327802	8.51%	1.266%
10	8.332	926	935	943	rBV	581384	1022537	26.54%	3.948%
11	9.160	1068	1076	1086	rVB	478765	864556	22.44%	3.338%
12	10.806	1349	1356	1364	rBV	259057	464169	12.05%	1.792%
13	13.256	1764	1773	1782	rBV	1394912	2107476	54.71%	8.137%
14	14.078	1906	1913	1923	rBV	388256	561623	14.58%	2.168%
15	14.631	1998	2007	2015	rVB3	456455	750636	19.48%	2.898%
16	15.477	2146	2151	2155	rVB	37537	48379	1.26%	0.187%
17	16.117	2252	2260	2272	rBV	1299467	1999999	51.92%	7.722%
18	16.334	2293	2297	2299	rBV2	59684	76494	1.99%	0.295%
19	16.358	2299	2301	2306	rVB3	33142	39256	1.02%	0.152%
20	17.122	2427	2431	2436	rBV	56713	75607	1.96%	0.292%
21	17.374	2467	2474	2480	rBV2	725364	1078200	27.99%	4.163%
22	17.750	2532	2538	2541	rBV8	19889	39348	1.02%	0.152%
23	17.862	2553	2557	2561	rBV	61076	74651	1.94%	0.288%
24	18.256	2620	2624	2631	rBV2	83724	139293	3.62%	0.538%
25	18.408	2646	2650	2656	rVB5	28523	38776	1.01%	0.150%
26	18.555	2670	2675	2680	rBV	48648	66780	1.73%	0.258%
27	19.184	2778	2782	2787	rVB	43621	50360	1.31%	0.194%
28	19.754	2876	2879	2885	rVB2	34033	39971	1.04%	0.154%
29	19.983	2912	2918	2926	rVB	2750827	3503920	90.95%	13.528%
30	20.289	2965	2970	2973	rBV2	33051	39583	1.03%	0.153%
31	21.287	3135	3140	3144	rBV5	25724	43923	1.14%	0.170%
32	21.634	3191	3199	3206	rBV	824129	1342568	34.85%	5.184%
33	23.303	3477	3483	3490	rVB2	95593	172102	4.47%	0.664%
34	24.819	3730	3741	3755	rBV2	468210	1332845	34.60%	5.146%

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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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-BG091115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

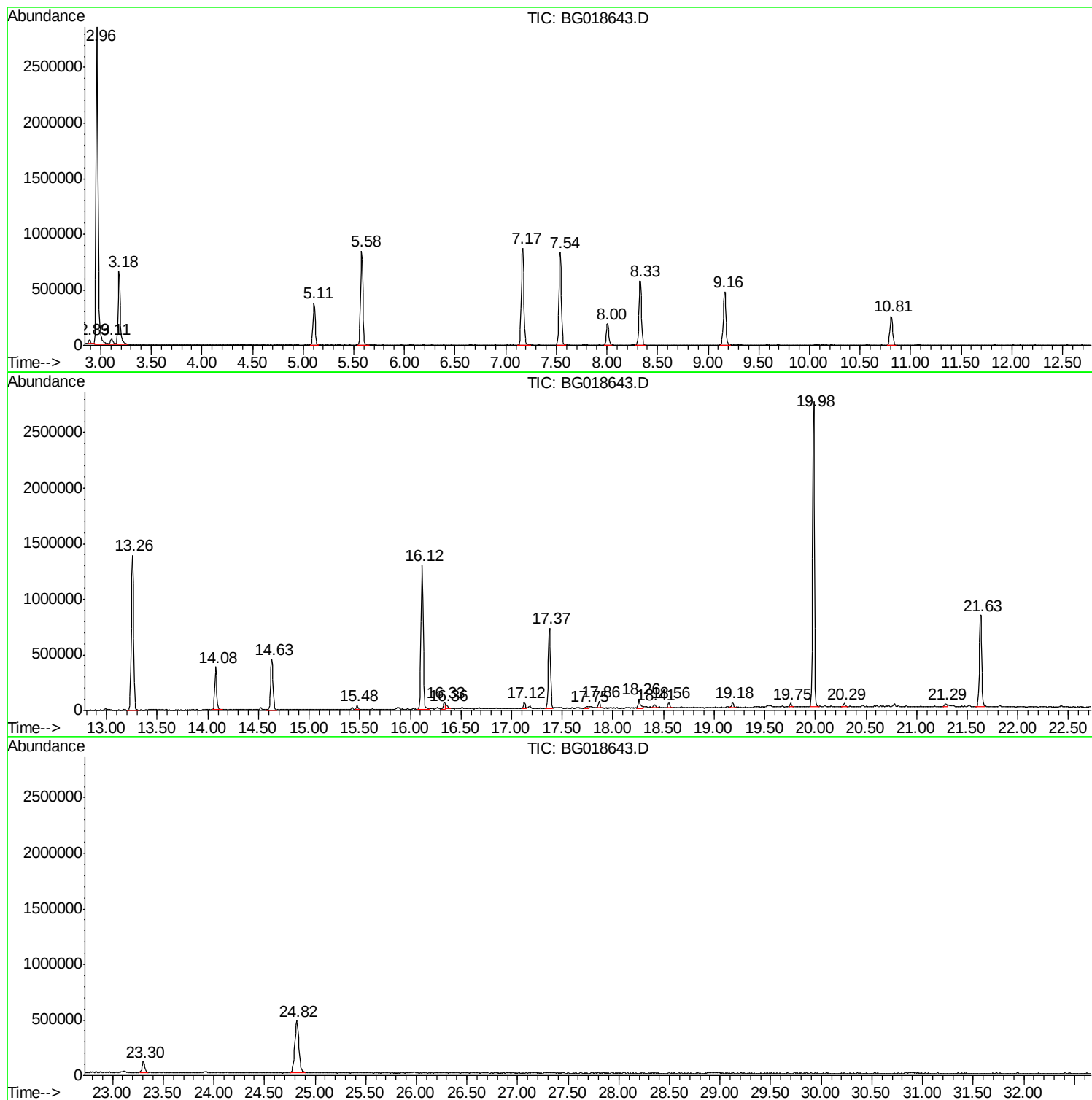
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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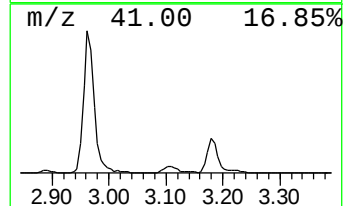
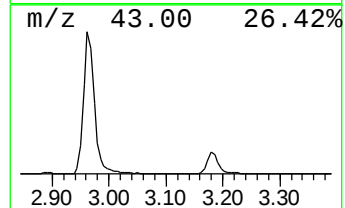
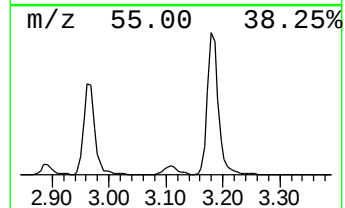
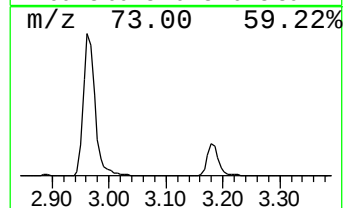
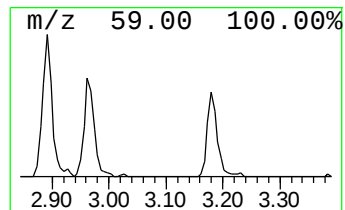
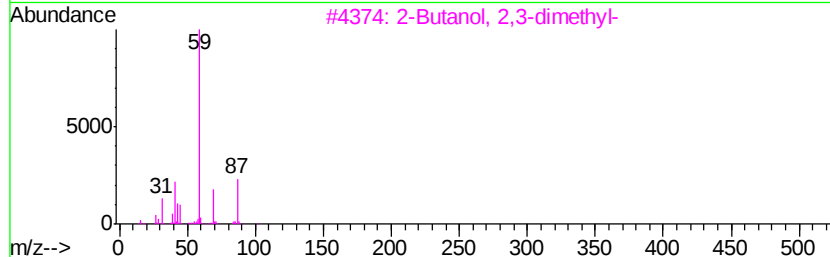
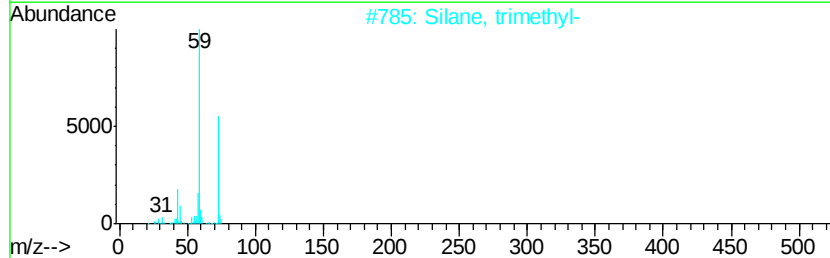
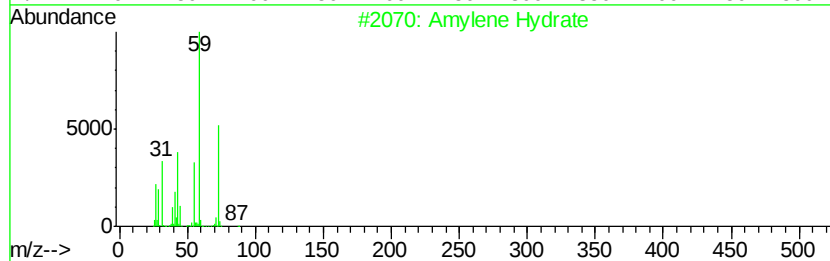
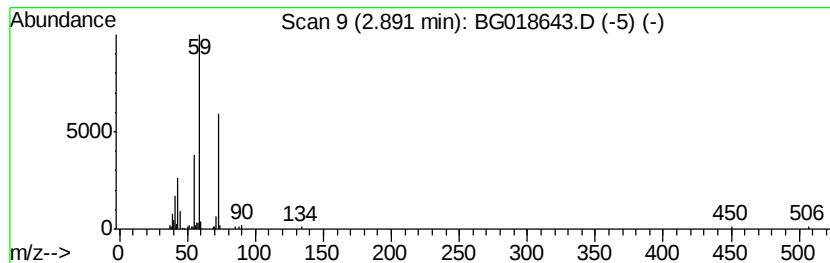
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Amylene Hydrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	2.63 ng	43080	1,4-Dichlorobenzene-d4	8.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene Hydrate	88	C5H12O	000075-85-4	78	
2	Silane, trimethyl-	74	C3H10Si	000993-07-7	50	
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	45	
4	3-Hexanol	102	C6H14O	000623-37-0	39	
5	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	38	



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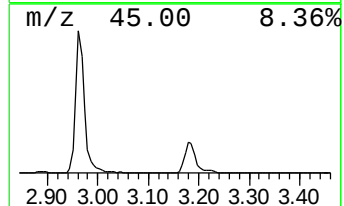
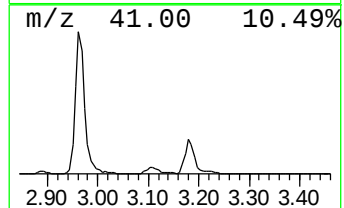
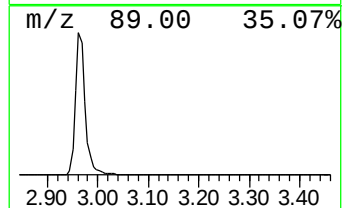
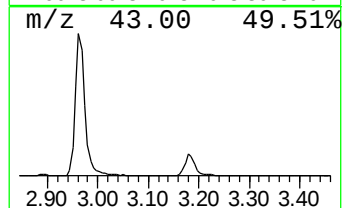
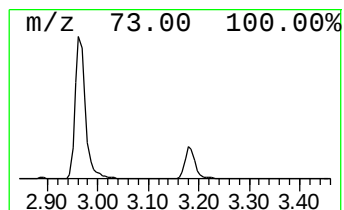
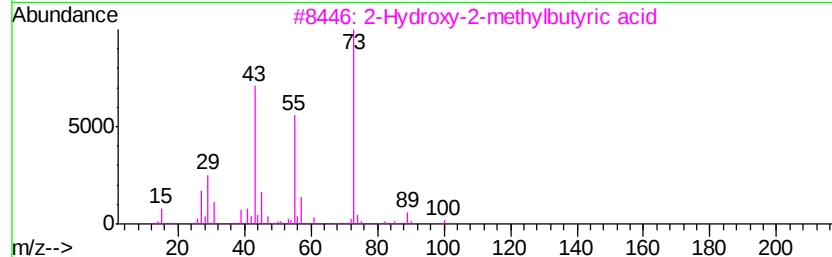
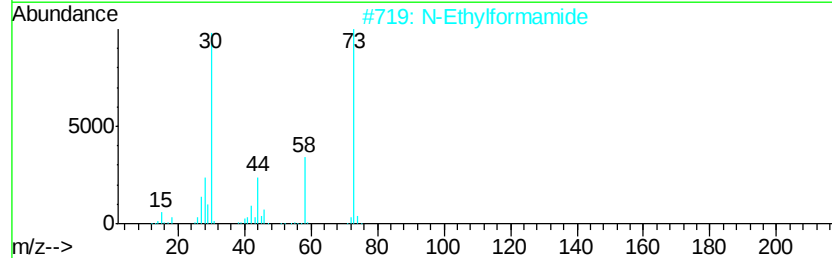
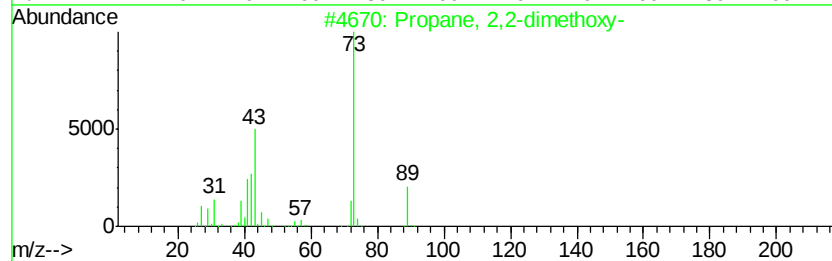
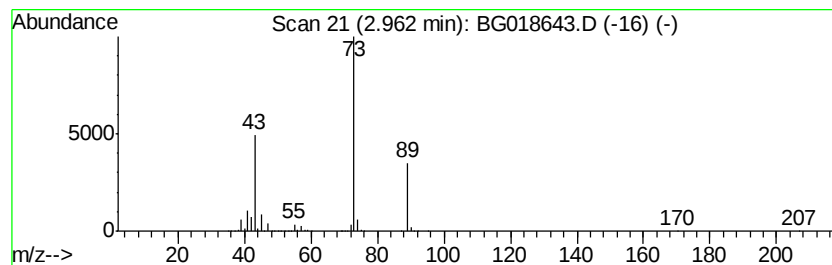
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.96 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.96	235.04 ng	3852380	1,4-Dichlorobenzene-d4	8.00

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		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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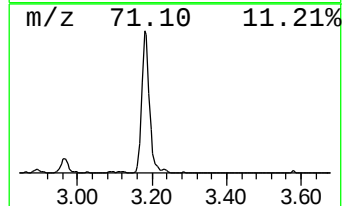
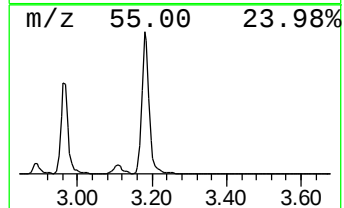
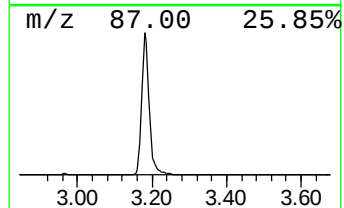
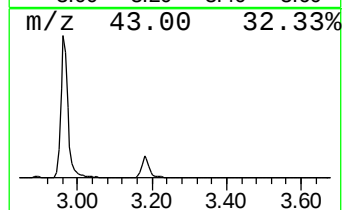
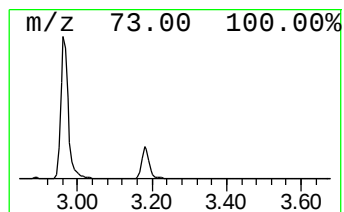
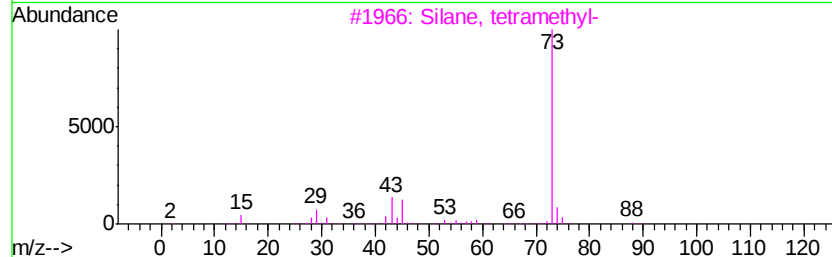
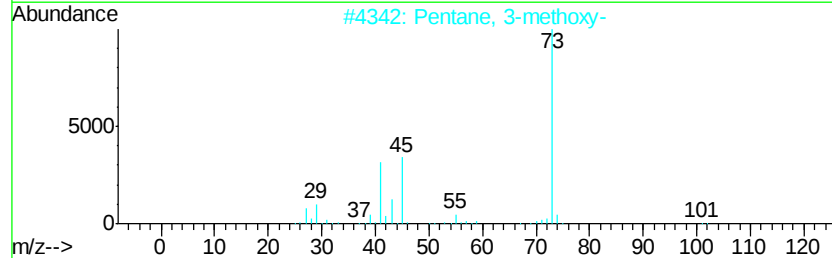
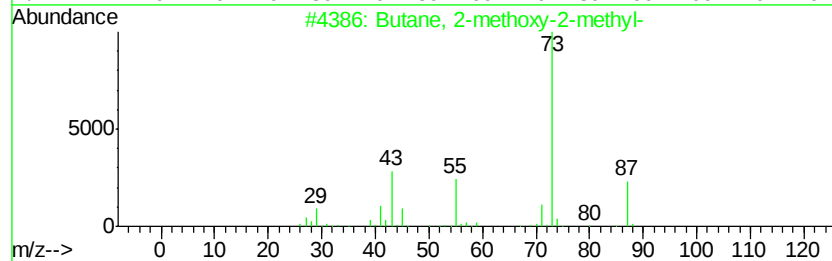
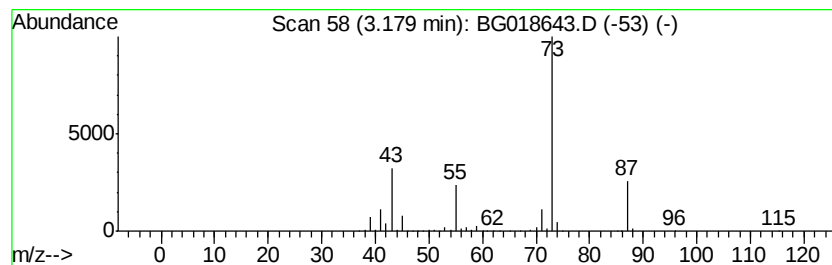
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	56.09 ng	919350	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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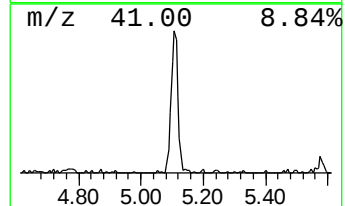
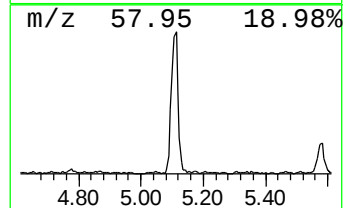
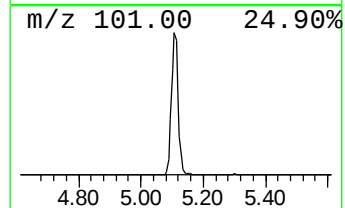
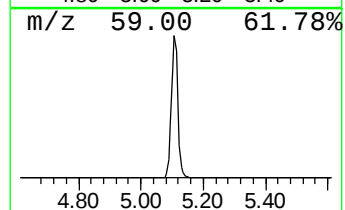
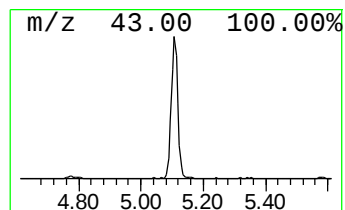
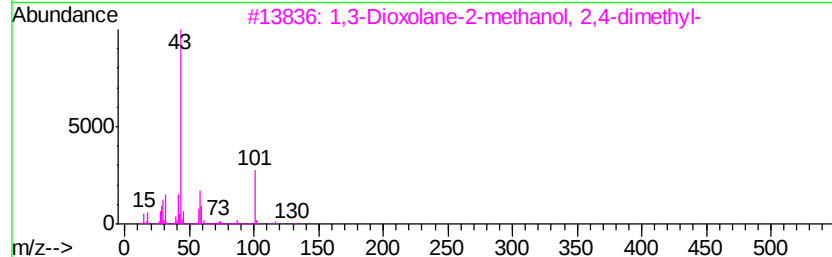
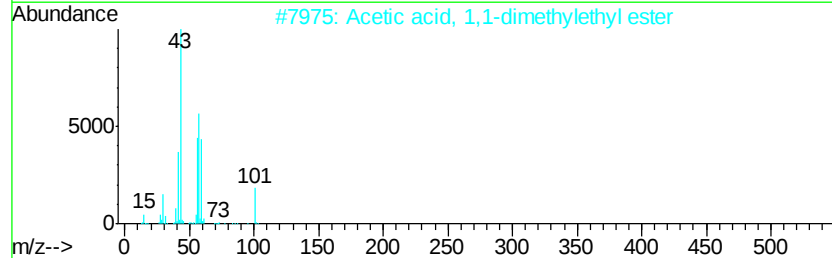
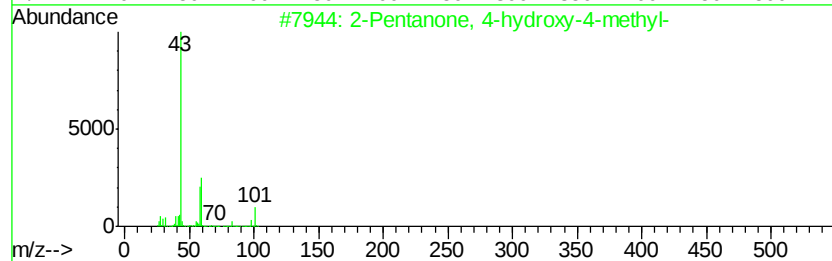
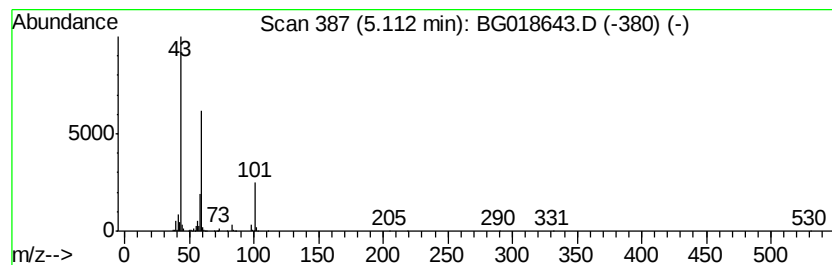
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	33.77 ng	553411	1,4-Dichlorobenzene-d4	8.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25	
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	



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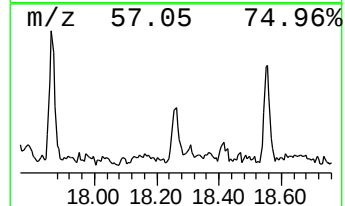
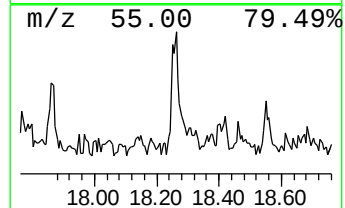
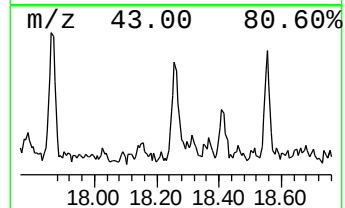
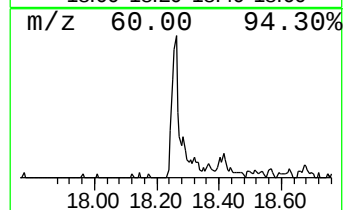
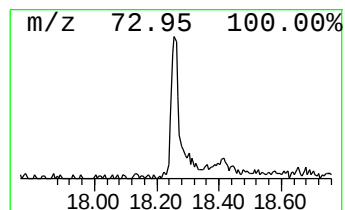
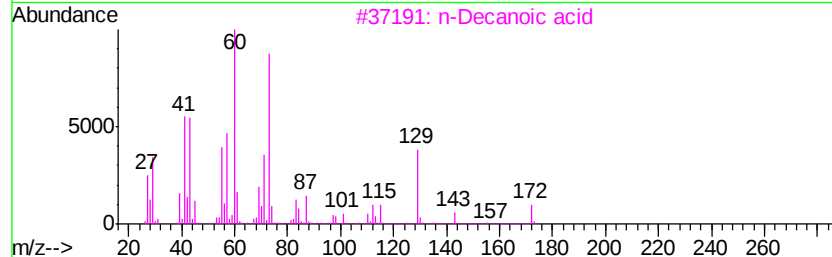
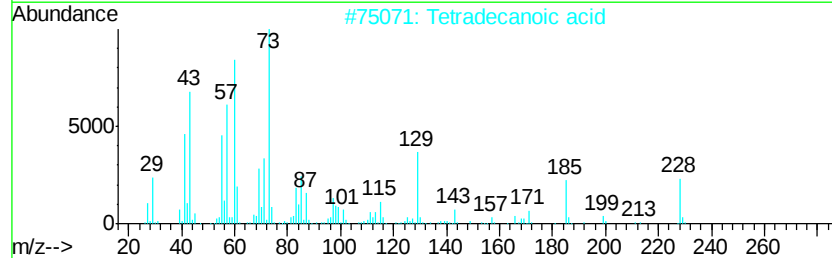
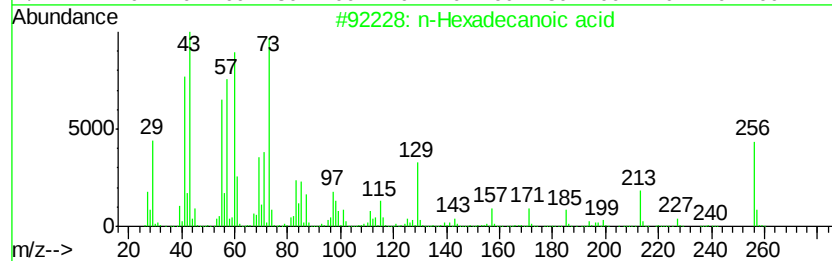
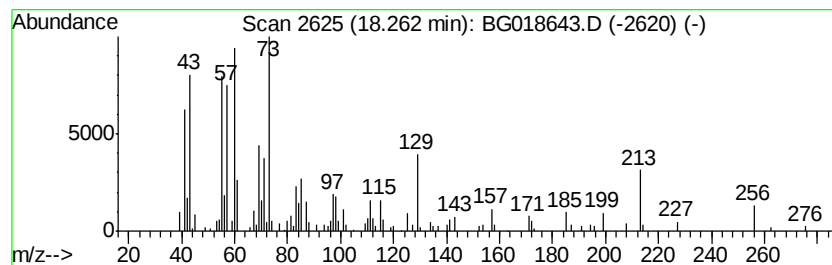
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.58 ng	139293	Phenanthrene-d10	17.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		n-Decanoic acid	172	C10H20O2	000334-48-5	62
4		Propyl 4,4-dimethyl-3-oxopentanoate	186	C10H18O3	077067-73-3	11
5		Tridecane	184	C13H28	000629-50-5	10



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ClientSampleId :
B-21

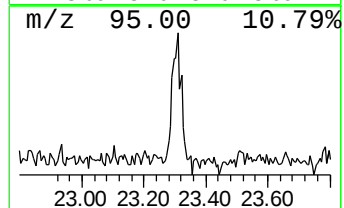
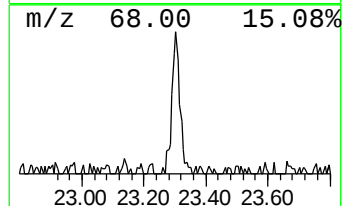
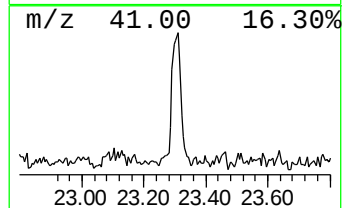
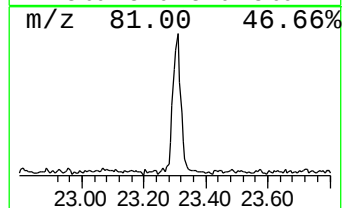
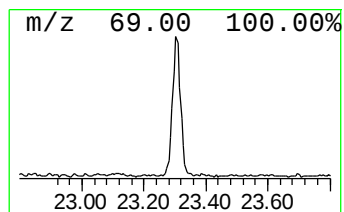
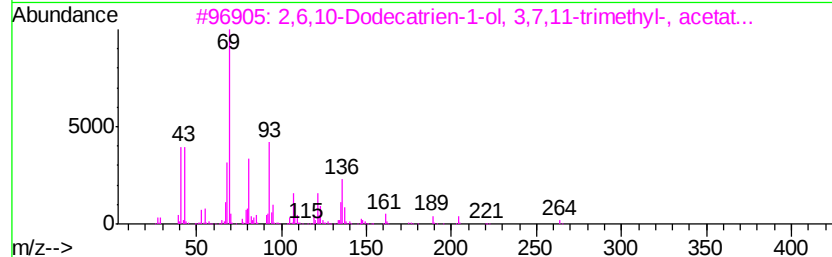
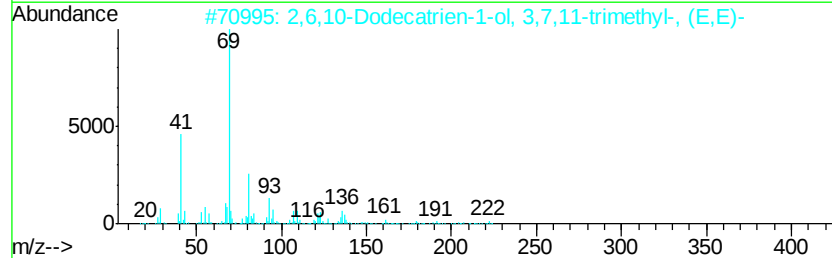
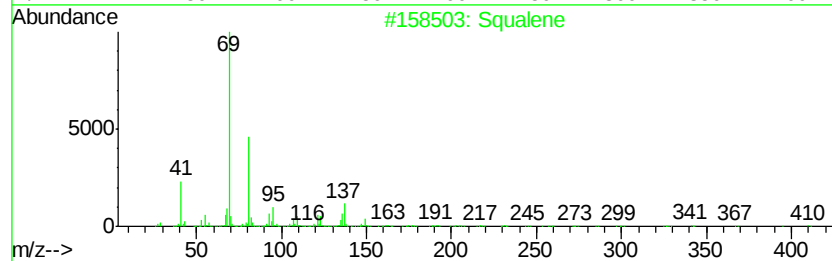
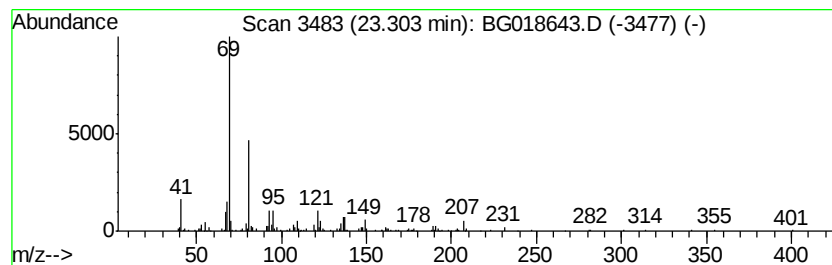
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	2.58 ng	172102	Perylene-d12	24.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	83
2		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	72
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
4		Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	64
5		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	58



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018643.D
Acq On : 11 Sep 2015 17:30
Operator : UM/IZ
Sample : G3612-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-21

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.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
Amylene Hydrate	2.89	2.6	ng	43080	1	8.00	327802	20.0
unknown2.96	2.96	235.0	ng	3852380	1	8.00	327802	20.0
Butane, 2-methoxy...	3.18	56.1	ng	919350	1	8.00	327802	20.0
2-Pentanone, 4-hy...	5.11	33.8	ng	553411	1	8.00	327802	20.0
n-Hexadecanoic acid	18.26	2.6	ng	139293	4	17.37	1078200	20.0
Squalene	23.30	2.6	ng	172102	6	24.82	1332850	20.0