

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
 Data File : BG019897.D
 Acq On : 4 Dec 2015 8:17
 Operator : UM/NP
 Sample : G4609-02
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-4-13.5-14.0-113015

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	2.993	21	26	46	rVV	1538361	2070085	77.20%	12.727%
2	3.140	46	51	60	rVV2	38141	77694	2.90%	0.478%
3	3.216	60	64	73	rVB	74415	104552	3.90%	0.643%
4	5.190	392	400	409	rBV	115763	175616	6.55%	1.080%
5	5.661	473	480	491	rBV	543345	840461	31.35%	5.167%
6	7.265	745	753	763	rBV	576837	987569	36.83%	6.072%
7	7.646	810	818	827	rBV	557742	931337	34.73%	5.726%
8	8.116	892	898	905	rBV	101706	170615	6.36%	1.049%
9	8.445	944	954	963	rVB	394824	675124	25.18%	4.151%
10	9.286	1089	1097	1106	rBV	354046	621635	23.18%	3.822%
11	10.937	1372	1378	1387	rVB	142964	259532	9.68%	1.596%
12	13.375	1786	1793	1803	rVB	1018162	1593565	59.43%	9.797%
13	14.198	1926	1933	1941	rBV	236063	349523	13.04%	2.149%
14	14.750	2020	2027	2037	rVB2	260005	419153	15.63%	2.577%
15	16.230	2271	2279	2289	rBV	941982	1400502	52.23%	8.610%
16	16.448	2311	2316	2319	rBV2	21526	31296	1.17%	0.192%
17	17.488	2485	2493	2501	rBV	353556	547897	20.43%	3.369%
18	18.369	2638	2643	2651	rBV	86978	123646	4.61%	0.760%
19	19.227	2784	2789	2795	rBV3	20237	31436	1.17%	0.193%
20	19.632	2854	2858	2868	rBV8	25618	49118	1.83%	0.302%
21	19.773	2878	2882	2887	rBV3	19532	31202	1.16%	0.192%
22	19.897	2900	2903	2910	rVB2	23629	33264	1.24%	0.205%
23	20.097	2931	2937	2942	rBV	2003924	2681284	100.00%	16.485%
24	20.302	2968	2972	2977	rBV2	24939	34361	1.28%	0.211%
25	20.778	3050	3053	3059	rVB	42387	61710	2.30%	0.379%
26	20.860	3061	3067	3073	rVV3	36382	62911	2.35%	0.387%
27	20.995	3086	3090	3094	rBV3	28688	48147	1.80%	0.296%
28	21.043	3095	3098	3102	rVB	51524	62856	2.34%	0.386%
29	21.113	3107	3110	3114	rVB3	25768	33844	1.26%	0.208%
30	21.366	3149	3153	3156	rBV5	19975	29904	1.12%	0.184%
31	21.401	3156	3159	3170	rVB2	84008	116879	4.36%	0.719%
32	21.560	3183	3186	3190	rVB	45282	54295	2.02%	0.334%
33	21.630	3194	3198	3202	rBV2	25505	39439	1.47%	0.242%
34	21.765	3215	3221	3230	rVB	433388	703202	26.23%	4.323%

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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	22.112	3276	3280	3285	rVB2	23943	35261	1.32%	0.217%
36	22.741	3383	3387	3393	rVB2	19728	33696	1.26%	0.207%
37	23.510	3512	3518	3528	rVB	56183	112482	4.20%	0.692%
38	25.050	3771	3780	3792	rVB2	224805	629960	23.49%	3.873%

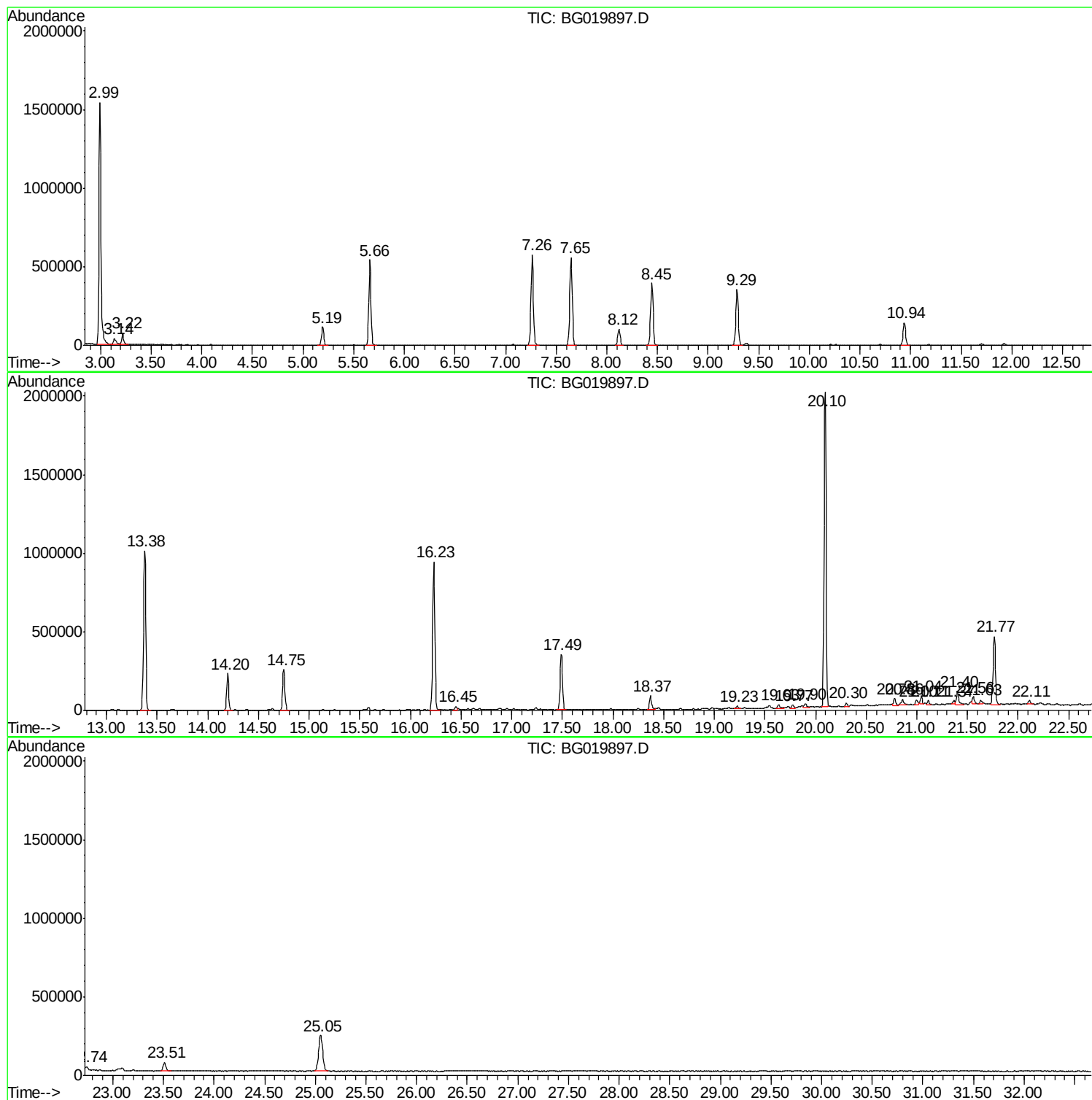
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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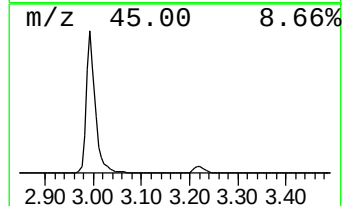
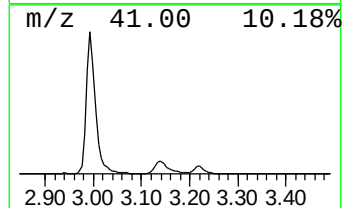
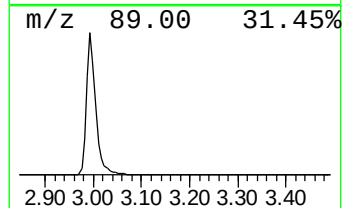
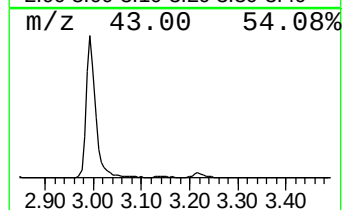
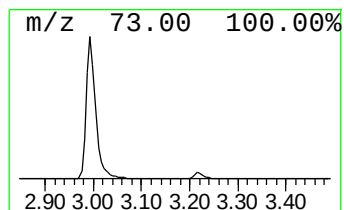
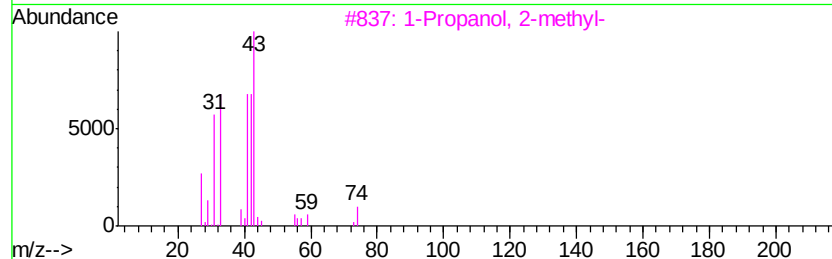
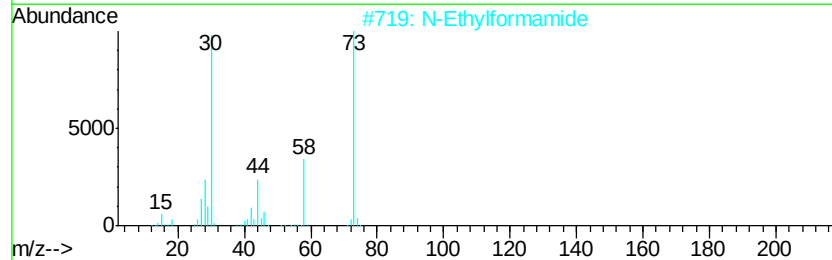
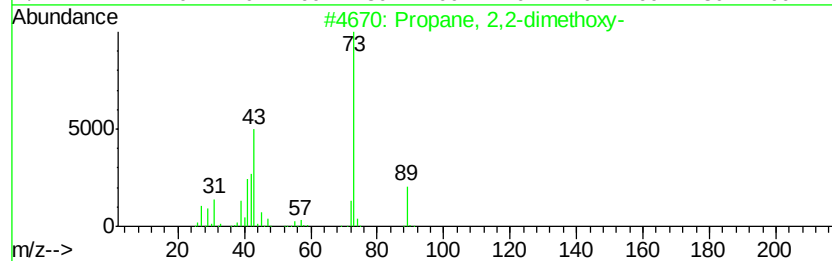
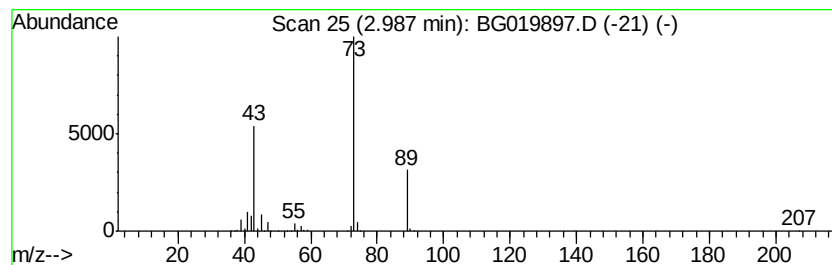
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	242.66 ng	2070090	1,4-Dichlorobenzene-d4	8.12

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



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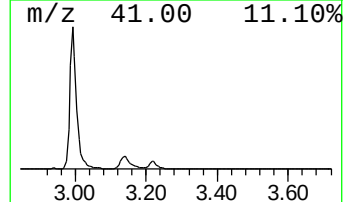
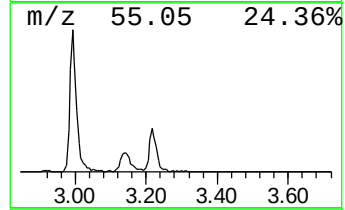
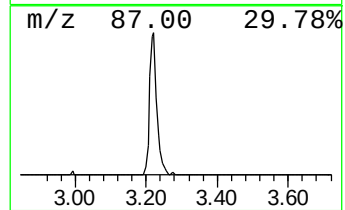
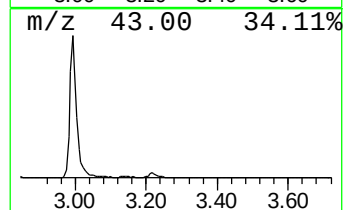
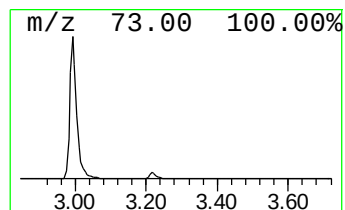
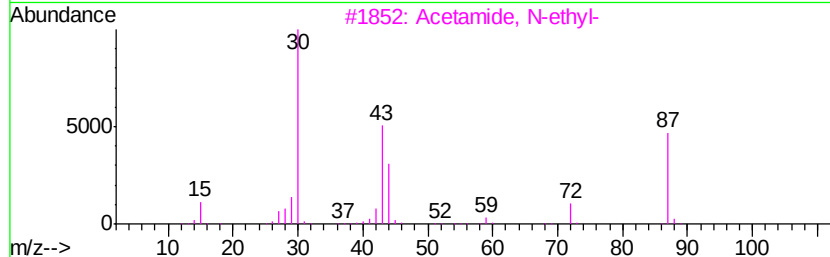
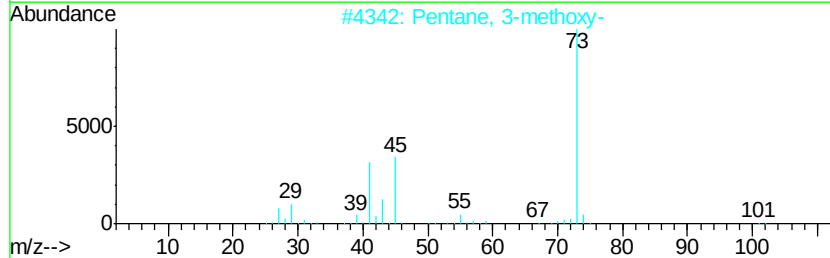
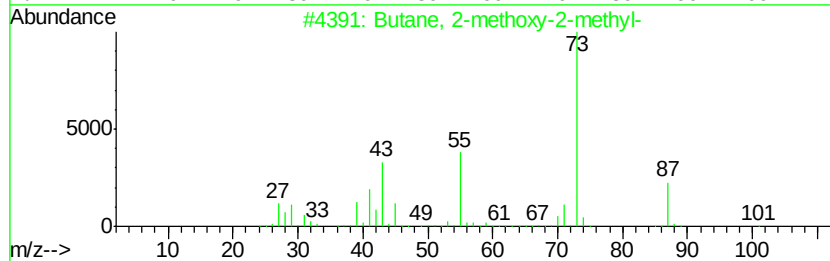
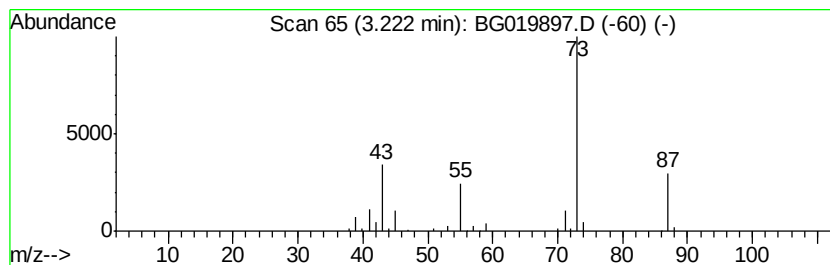
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	12.26 ng	104552	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
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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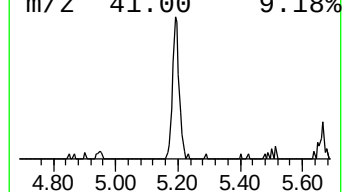
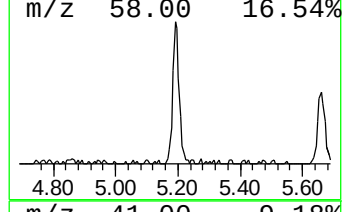
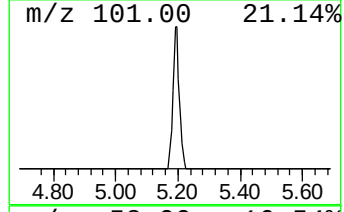
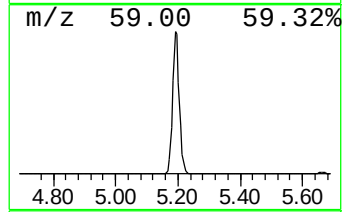
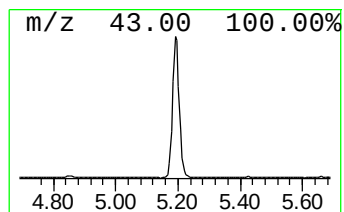
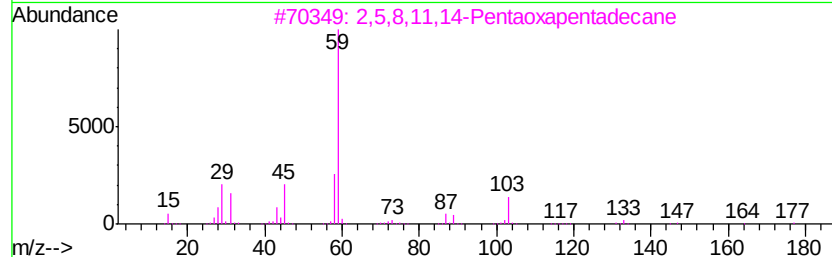
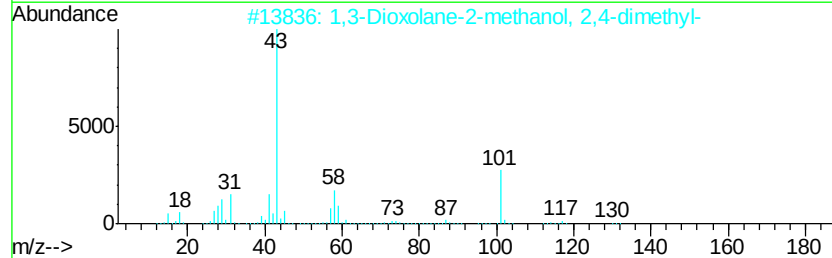
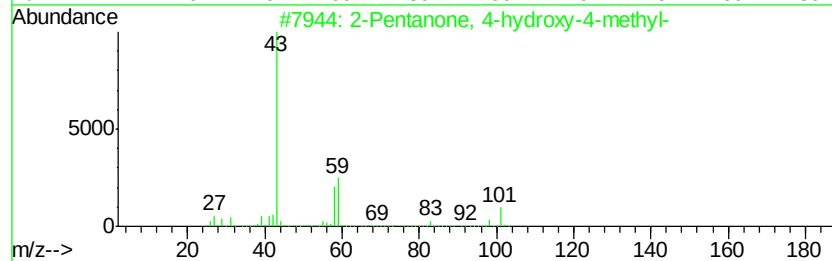
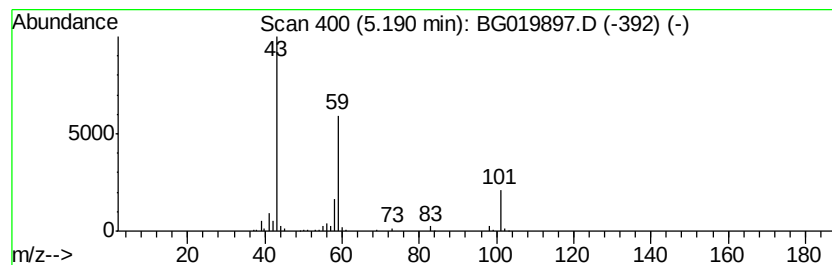
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	20.59 ng	175616	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	72
2		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3		2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	25
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5		2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23



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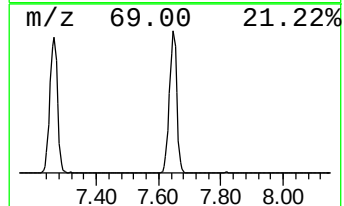
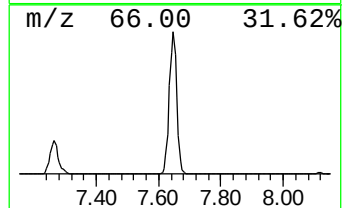
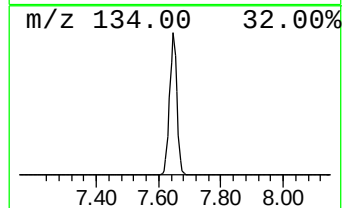
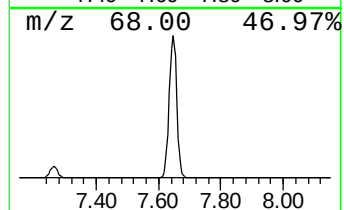
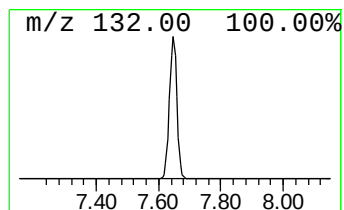
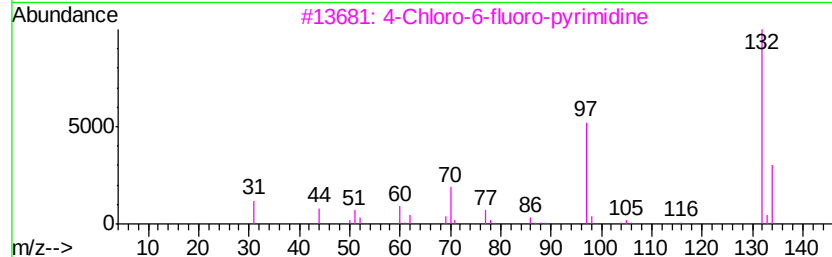
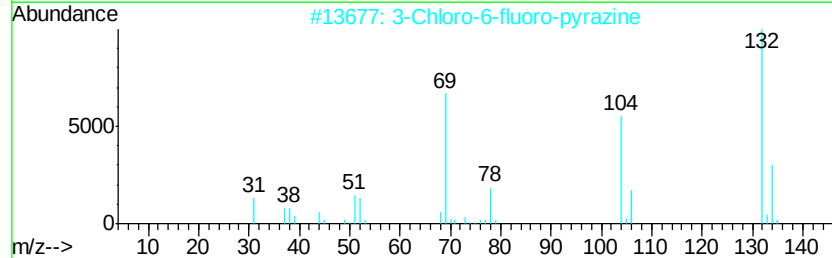
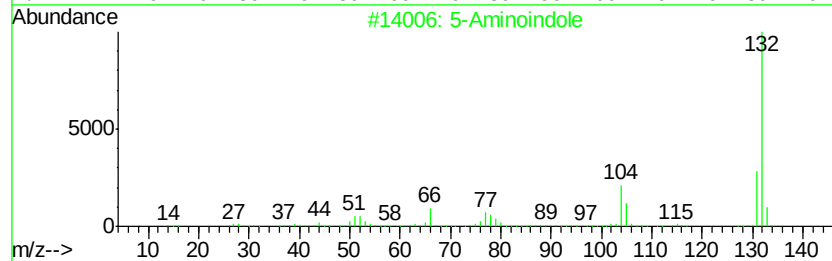
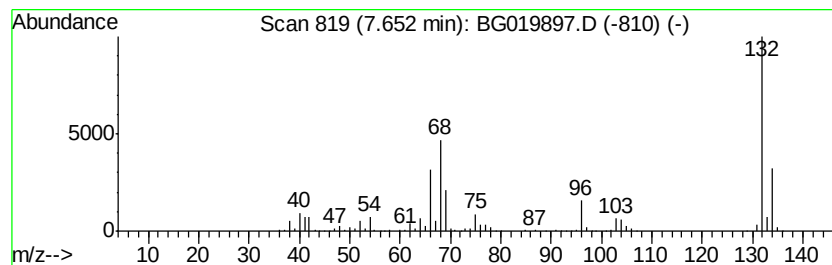
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	109.17 ng	931337	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	40
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13



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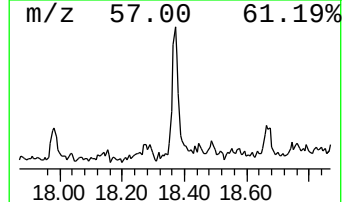
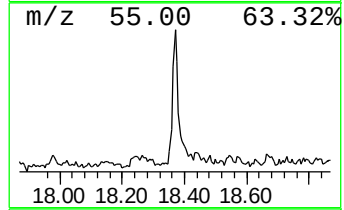
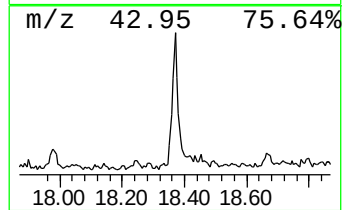
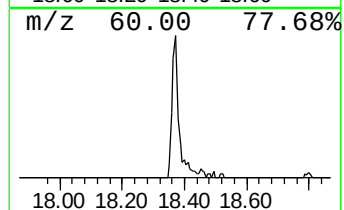
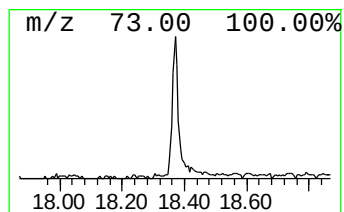
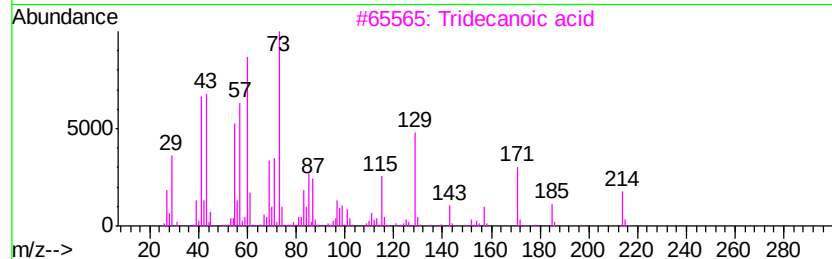
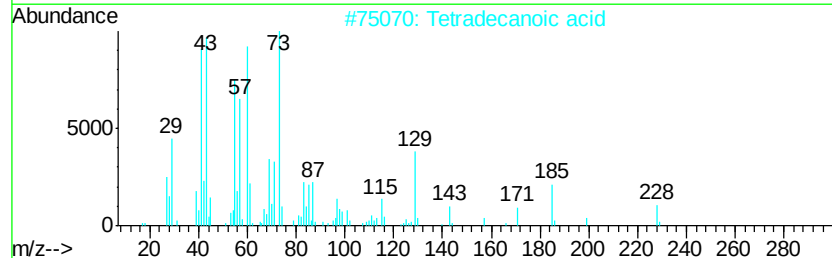
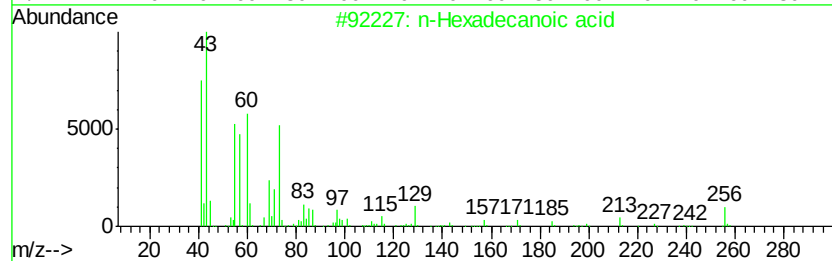
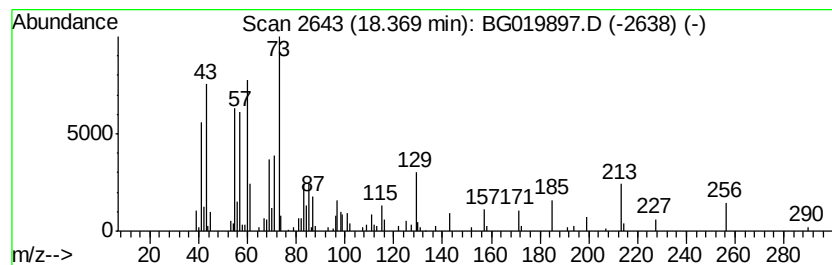
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.37	4.51 ng	123646	Phenanthrene-d10	17.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019897.D
Acq On : 4 Dec 2015 8:17
Operator : UM/NP
Sample : G4609-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

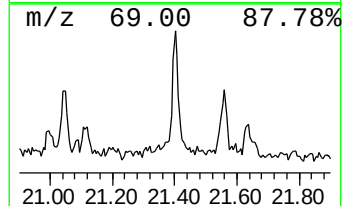
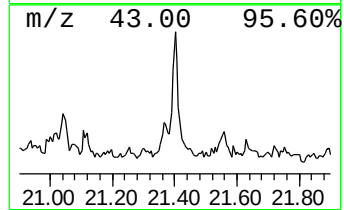
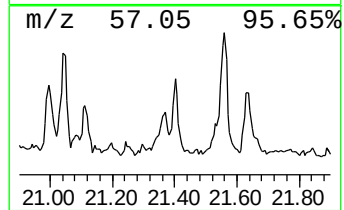
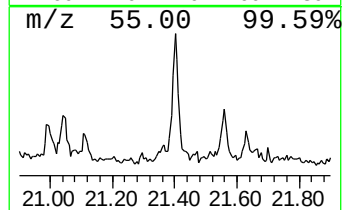
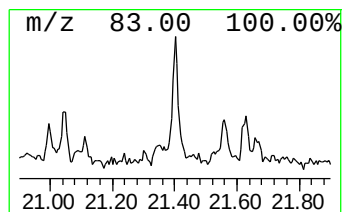
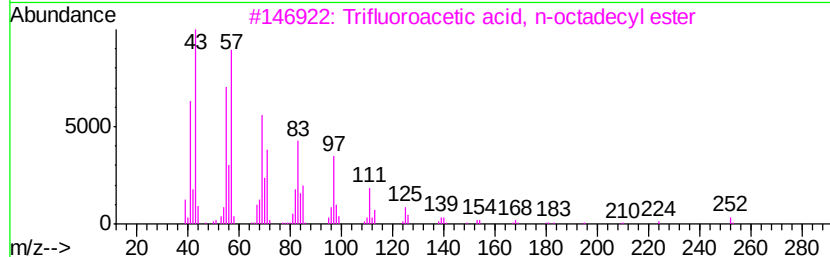
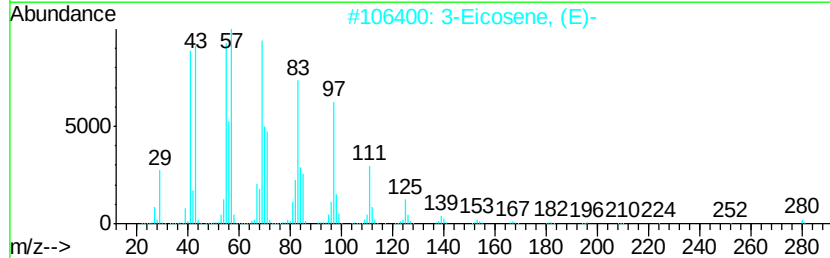
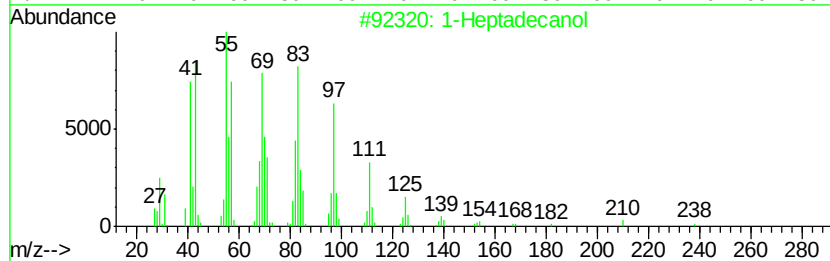
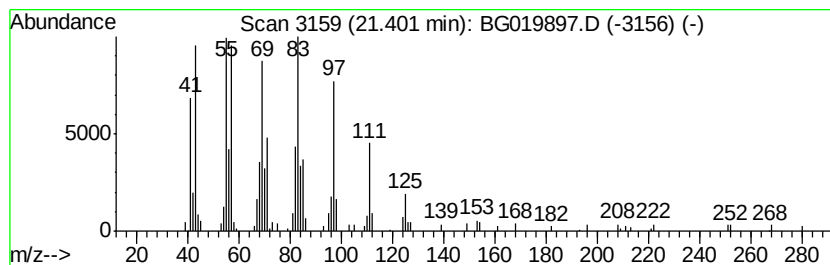
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SB-4-13.5-14.0-113015

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 1-Heptadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	3.32 ng	116879	Chrysene-d12	21.77
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptadecanol	256 C17H36O	001454-85-9	87
2	3-Eicosene, (E)-	280 C20H40	074685-33-9	83
3	Trifluoroacetic acid, n-octadecyl...	366 C20H37F3O2	079392-43-1	83
4	1-Eicosanol	298 C20H42O	000629-96-9	81
5	1-Hexadecanol	242 C16H34O	036653-82-4	80



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120315\
Data File : BG019897.D
Acq On : 4 Dec 2015 8:17
Operator : UM/NP
Sample : G4609-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-4-13.5-14.0-113015

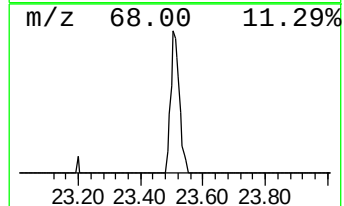
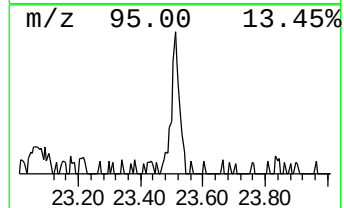
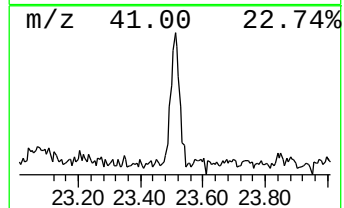
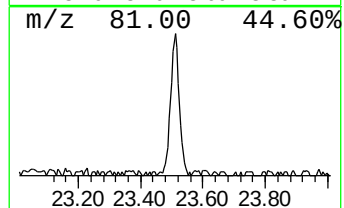
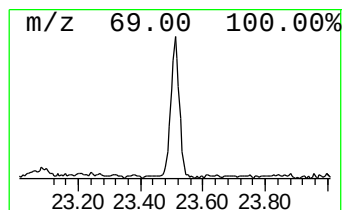
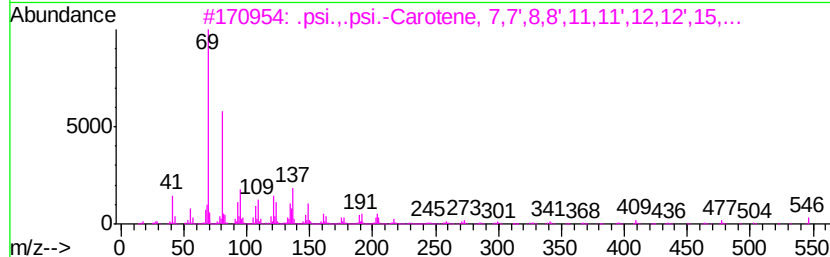
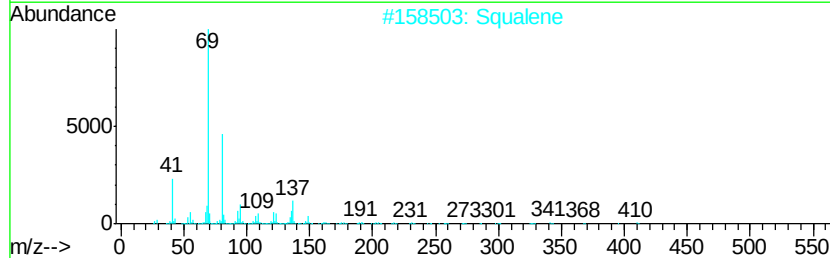
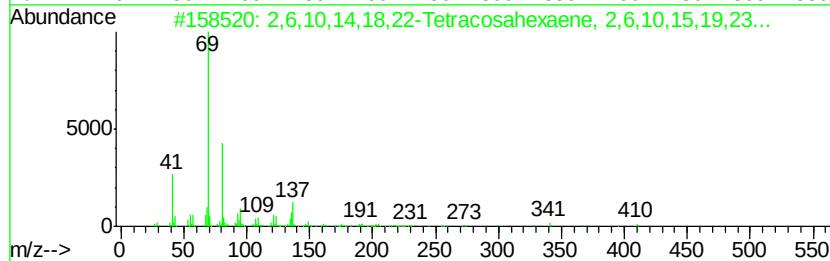
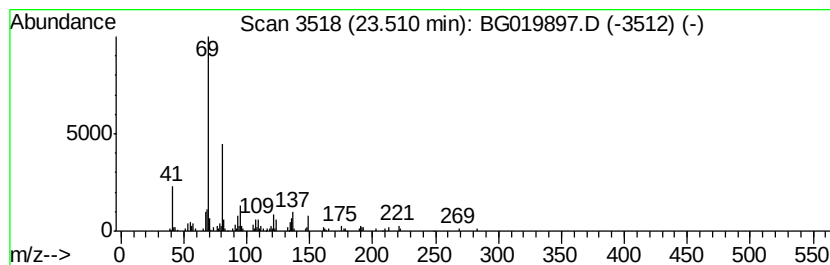
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.51	3.57 ng	112482	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	91		
2	Squalene	410	C30H50	007683-64-9	90		
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83		
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80		
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74		



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120315\
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Operator : UM/NP
Sample : G4609-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-4-13.5-14.0-113015

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...	2.99	242.7	ng	2070090	1	8.12	170615	20.0
Butane, 2-methoxy...	3.22	12.3	ng	104552	1	8.12	170615	20.0
2-Pentanone, 4-hy...	5.19	20.6	ng	175616	1	8.12	170615	20.0
unknown7.65	7.65	109.2	ng	931337	1	8.12	170615	20.0
n-Hexadecanoic acid	18.37	4.5	ng	123646	4	17.49	547897	20.0
1-Heptadecanol	21.40	3.3	ng	116879	5	21.77	703202	20.0
2,6,10,14,18,22-T...	23.51	3.6	ng	112482	6	25.05	629960	20.0