LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016251.D
Acq On : 7 Apr 2015 11:57
Operator : TP/IZ
Sample : G1775-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-021

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-BG040615.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	2.799	14	19	28	rBV	145914	228100	5.64%	0.902%
2	2.875	28	32	38	rVB	125088	135323	3.35%	0.535%
3	4.814	356	362	370	rBV	151070	211899	5.24%	0.837%
4	5.278	435	441	452	rBV	1234572	1781204	44.04%	7.040%
5	6.876	704	713	726	rBV	1322285	2107371	52.10%	8.329%
6	7.229	766	773	783	rBV	1275647	1999895	49.44%	7.904%
7	7.699	846	853	859	rBV	261950	391740	9.68%	1.548%
8	8.016	900	907	915	rBV	905010	1412360	34.92%	5.582%
9	8.856	1041	1050	1057	rBV	749533	1216341	30.07%	4.807%
10	10.484	1320	1327	1334	rBV	388092	642782	15.89%	2.540%
11	11.806	1546	1552	1559	rVB	29178	46979	1.16%	0.186%
12	12.957	1741	1748	1759	rVB	2034733	2900491	71.71%	11.463%
13	13.792	1885	1890	1899	rVB	84494	113859	2.81%	0.450%
14	14.338	1976	1983	1992	rVB2	644468	948380	23.45%	3.748%
15	15.695	2209	2214	2221	rVB	149455	191547	4.74%	0.757%
16	15.825	2230	2236	2243	rBV	1447072	1989253	49.18%	7.862%
17	17.076	2443	2449	2459	rVB2	829182	1176395	29.08%	4.649%
18	17.975	2597	2602	2611	rBV	150686	230737	5.70%	0.912%
19	19.262	2816	2821	2830	rBV	35467	65873	1.63%	0.260%
20	19.708	2891	2897	2908	rBV	3352967	4044972	100.00%	15.987%
21	20.966	3107	3111	3123	rBV	497596	700112	17.31%	2.767%
22	21.254	3155	3160	3170	rVV	1046356	1251531	30.94%	4.946%
23	21.859	3257	3263	3272	rBV10	19311	46621	1.15%	0.184%
24	22.429	3355	3360	3370	rVB	137713	197780	4.89%	0.782%
25	23.498	3535	3542	3554	rVB2	622596	1172725	28.99%	4.635%
26	24.127	3643	3649	3659	rBV2	37149	97886	2.42%	0.387%

Sum of corrected areas: 25302156

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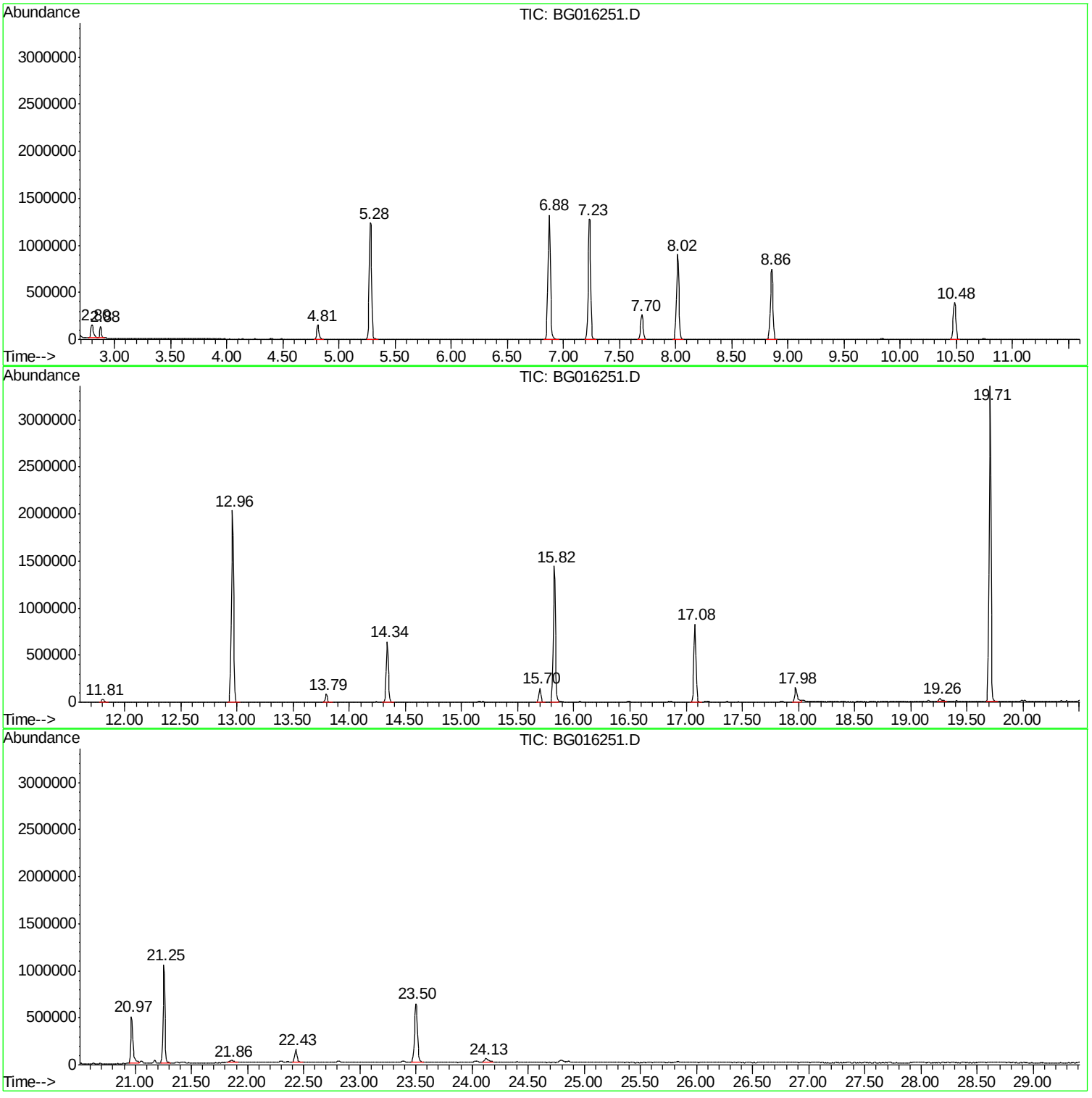
ClientSampleId : FS-021

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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Sample : G1775-04
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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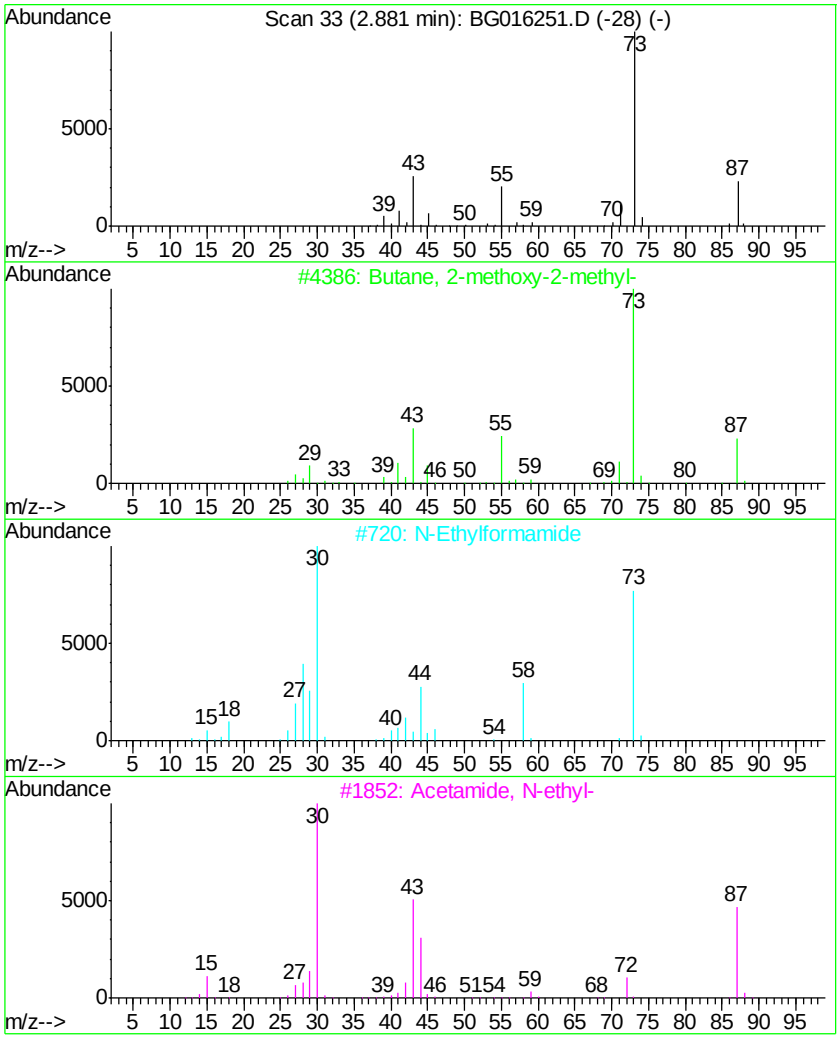
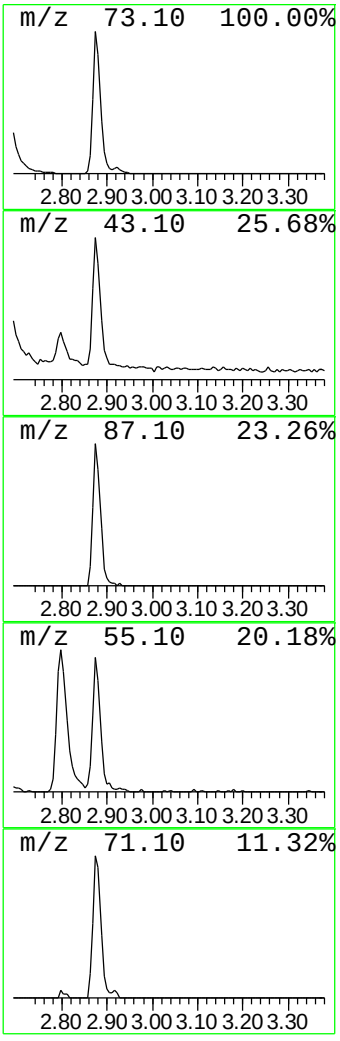
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	6.91 ng	135323	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7





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Acq On : 7 Apr 2015 11:57
Operator : TP/IZ
Sample : G1775-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-021

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

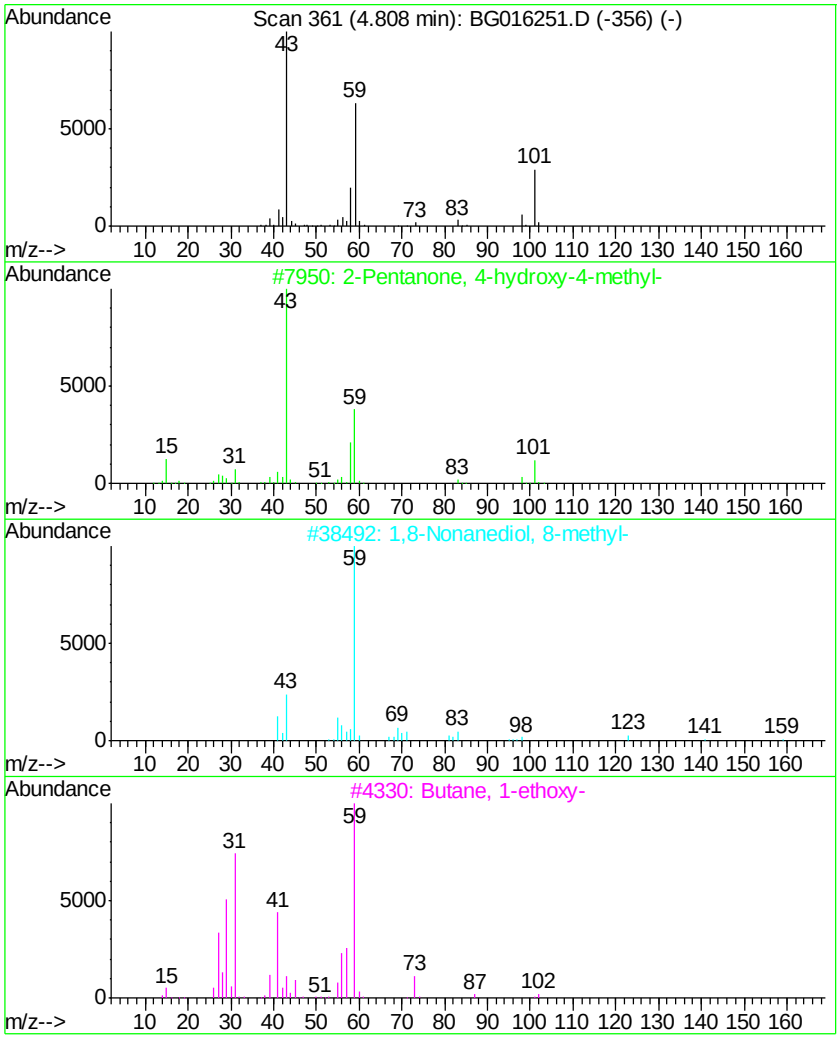
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

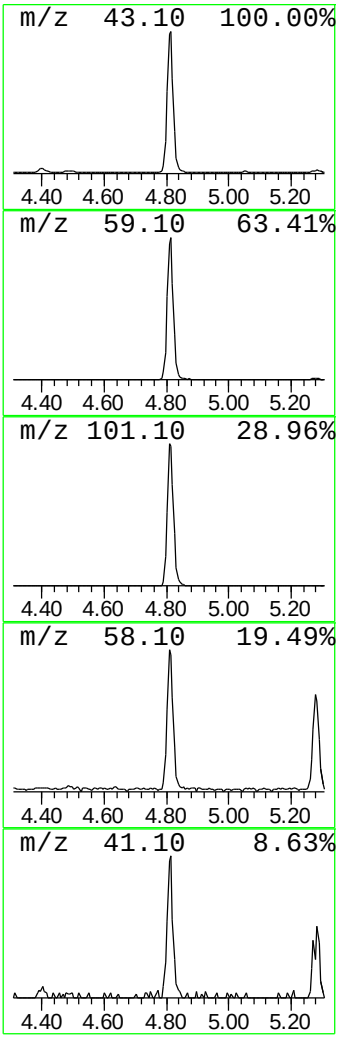
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	10.82 ng	211899	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016251.D
Acq On : 7 Apr 2015 11:57
Operator : TP/IZ
Sample : G1775-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-021

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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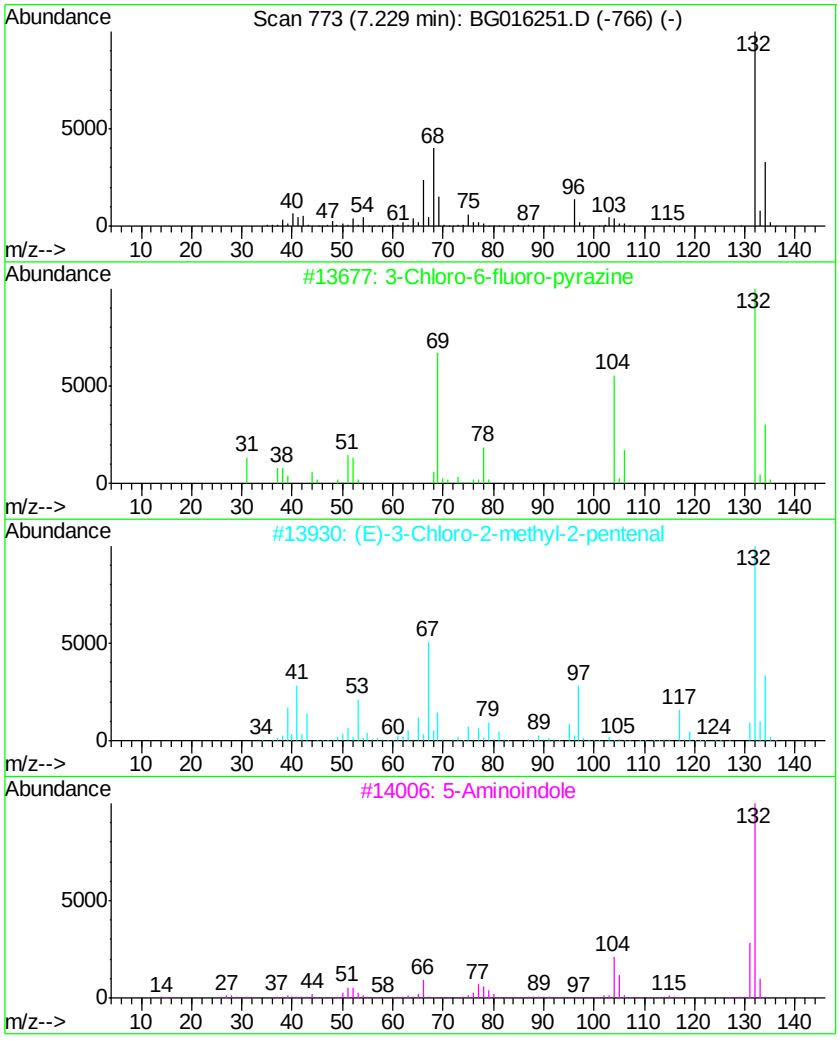
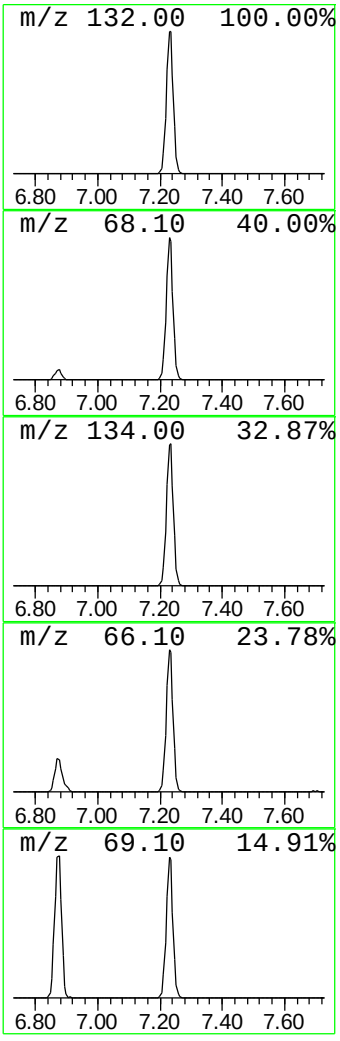
Peak Number 4 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	102.10 ng	1999900	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Operator : TP/IZ
Sample : G1775-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-021

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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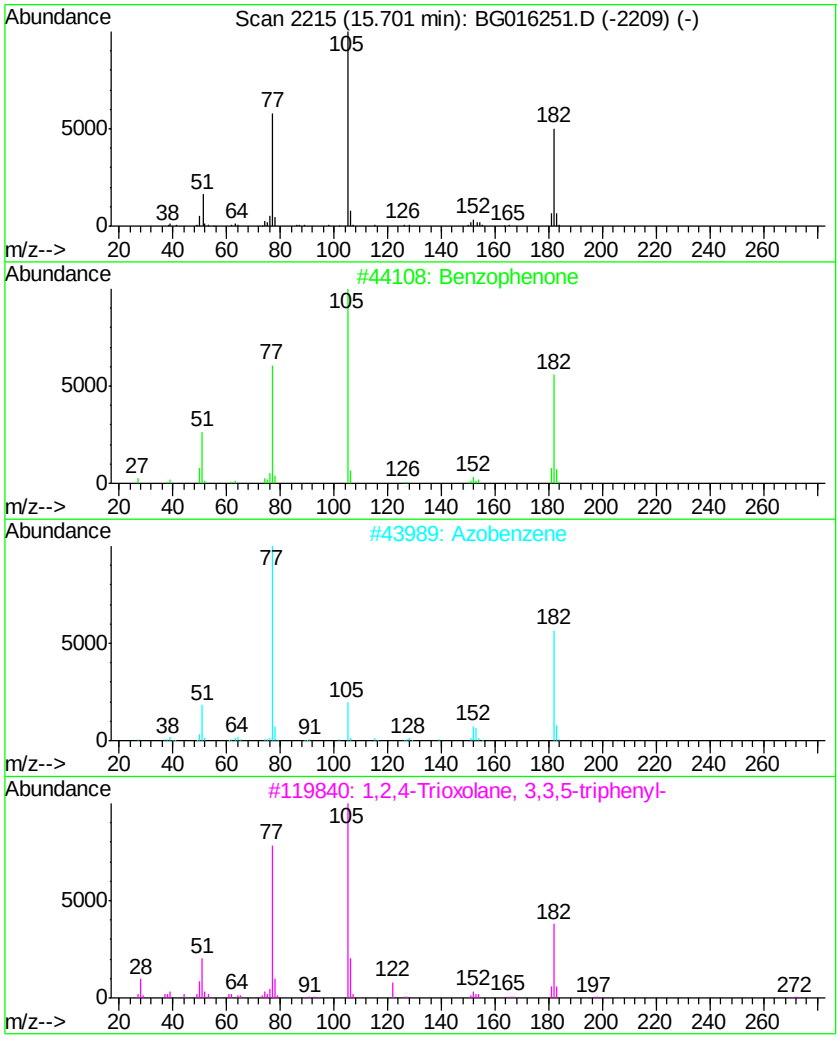
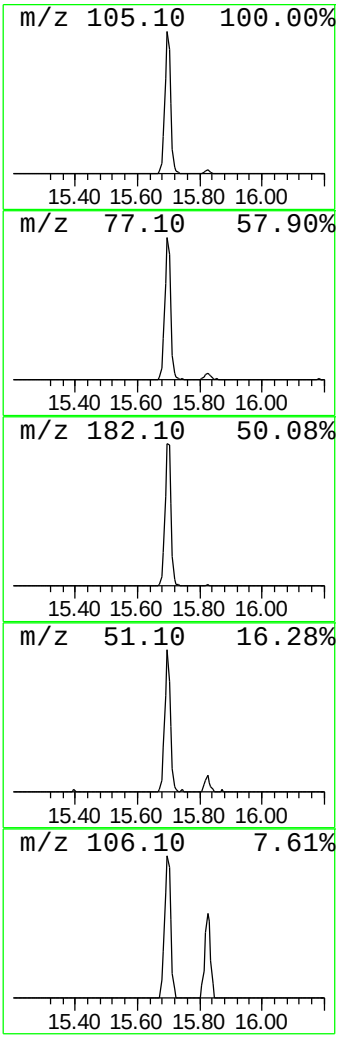
Peak Number 6 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	4.04 ng	191547	Acenaphthene-d10	14.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	72
3	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
4	Benzopinacol	366	C26H22O2	000464-72-2	50
5	Methyl benzillate	242	C15H14O3	000076-89-1	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040615\
Data File : BG016251.D
Acq On : 7 Apr 2015 11:57
Operator : TP/IZ
Sample : G1775-04
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FS-021

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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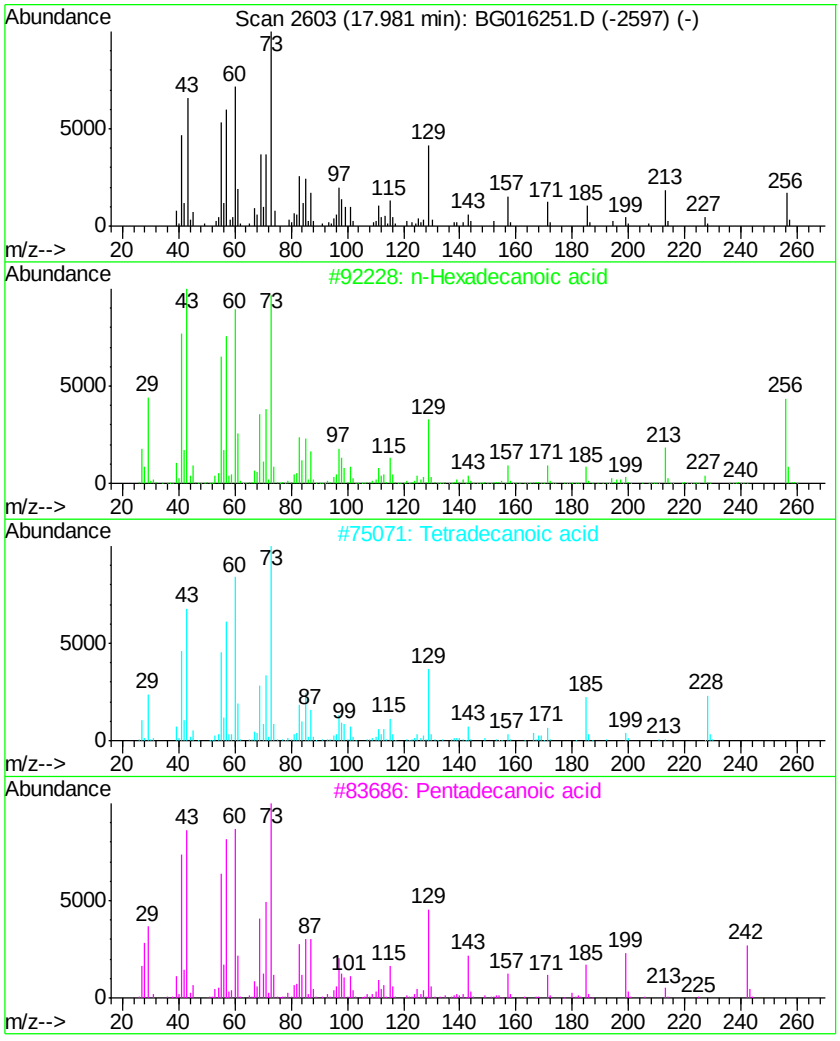
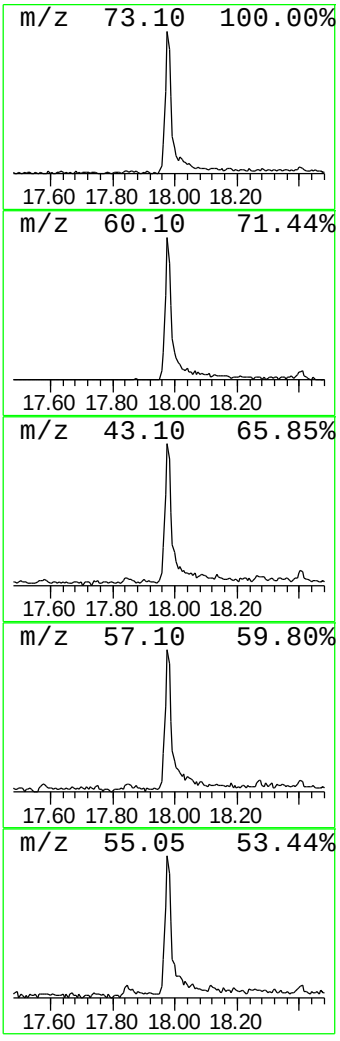
Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	3.92 ng	230737	Phenanthrene-d10	17.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Instrument : BNA_G
ClientSampleId : FS-021

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

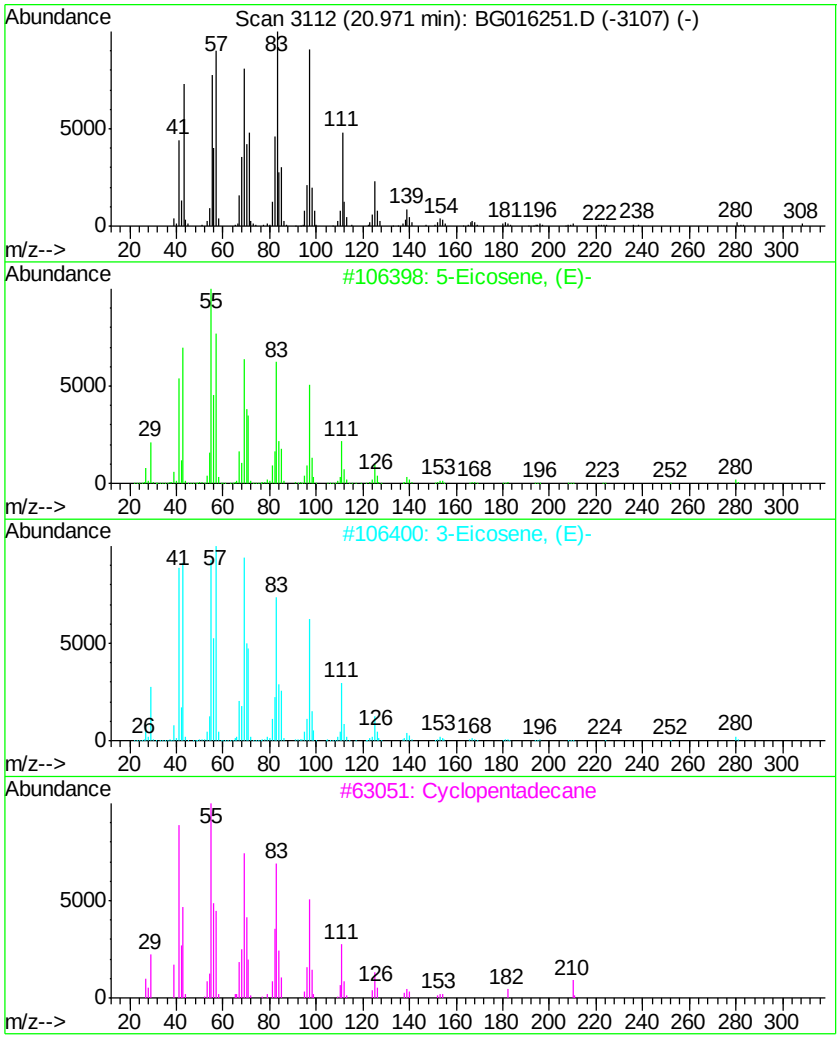
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

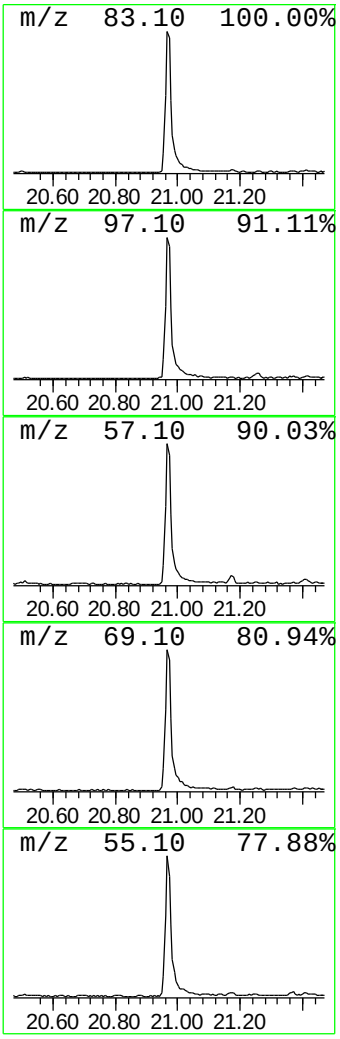
****

Peak Number 8 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	11.19 ng	700112	Chrysene-d12	21.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Cyclopentadecane	210	C15H30	000295-48-7	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	Cyclohexadecane	224	C16H32	000295-65-8	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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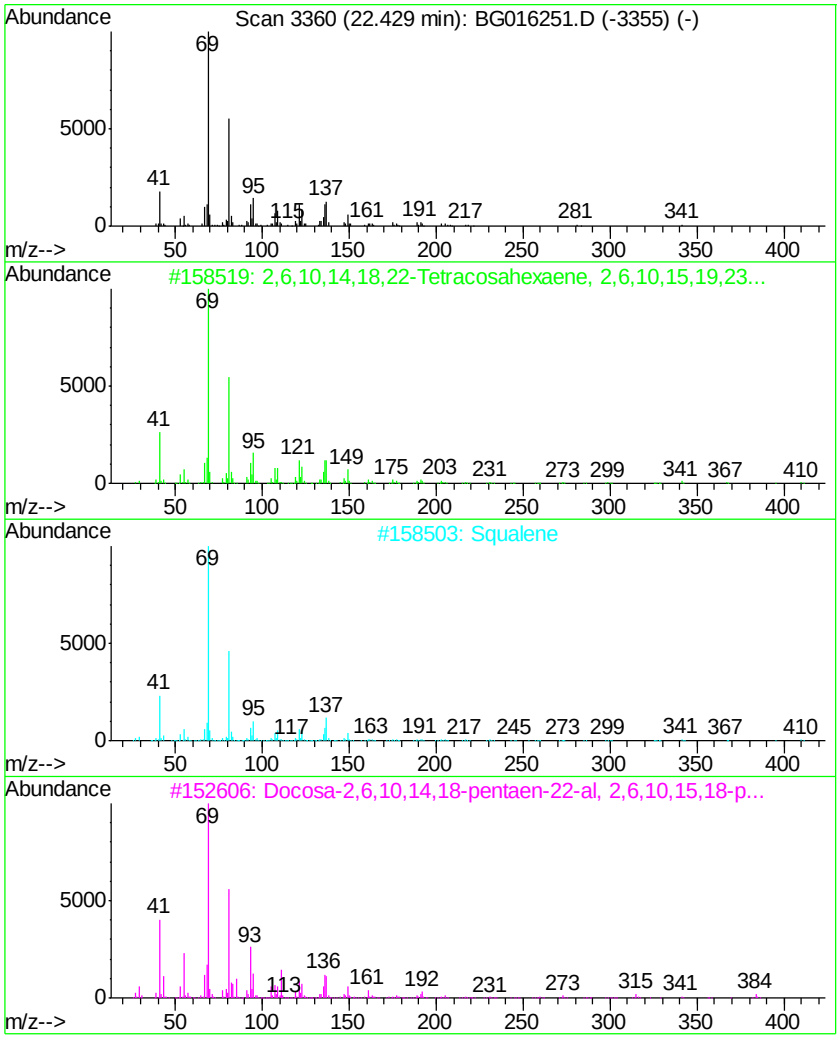
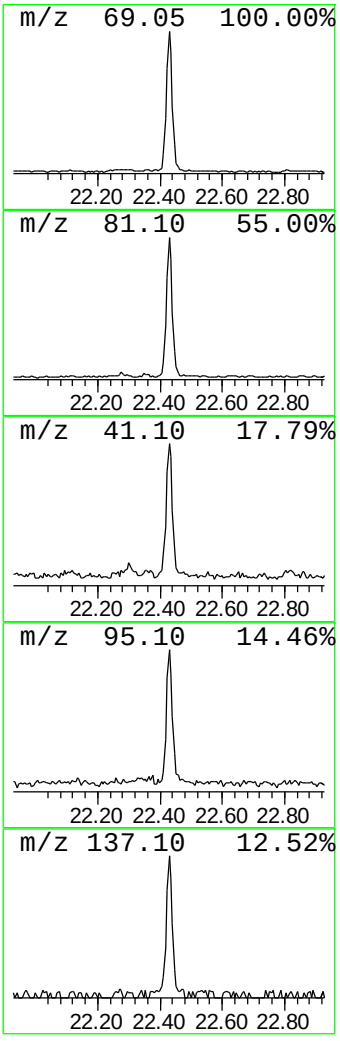
Peak Number 9 2,6,10,14,18,22-Tetracosahe... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.43	3.37 ng	197780	Perylene-d12	23.50

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	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	80
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.88	6.9	ng	135323	1	7.70	391740	20.0
2-Pentanone, 4-hy...	4.81	10.8	ng	211899	1	7.70	391740	20.0
unknown7.23	7.23	102.1	ng	1999900	1	7.70	391740	20.0
Benzophenone	15.70	4.0	ng	191547	3	14.34	948380	20.0
n-Hexadecanoic acid	17.98	3.9	ng	230737	4	17.08	1176400	20.0
5-Eicosene, (E)-	20.97	11.2	ng	700112	5	21.25	1251530	20.0
2,6,10,14,18,22-T...	22.43	3.4	ng	197780	6	23.50	1172730	20.0