LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022616\
Data File : BG021094.D
Acq On : 27 Feb 2016 1:24
Operator : UM/SJ
Sample : H1558-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S9

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-BG022616.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	2.950	12	19	37	rVB	34671	103336	19.75%	3.826%
2	3.096	38	44	62	rVV	133264	211561	40.44%	7.833%
3	3.237	62	68	78	rVV	32379	73592	14.07%	2.725%
4	5.264	407	413	420	rBB	20041	29616	5.66%	1.096%
5	5.723	485	491	498	rBB	96682	151796	29.01%	5.620%
6	7.315	755	762	769	rBB	103091	168862	32.28%	6.252%
7	7.697	821	827	834	rBB	99540	165822	31.70%	6.139%
8	8.173	902	908	913	rBB	17766	28866	5.52%	1.069%
9	8.496	956	963	970	rBB	71081	121112	23.15%	4.484%
10	9.336	1099	1106	1112	rBB	61071	105143	20.10%	3.893%
11	10.981	1380	1386	1393	rBB2	23522	41555	7.94%	1.538%
12	13.408	1792	1799	1806	rBB	177733	256877	49.10%	9.510%
13	14.225	1933	1938	1943	rBB	15618	21807	4.17%	0.807%
14	14.777	2027	2032	2038	rBB2	42461	62501	11.95%	2.314%
15	15.605	2169	2173	2177	rBB	5402	6207	1.19%	0.230%
16	16.252	2276	2283	2290	rBB3	153897	222929	42.61%	8.253%
17	16.463	2315	2319	2322	rBV	5500	7056	1.35%	0.261%
18	17.509	2492	2497	2504	rVB	57169	86090	16.46%	3.187%
19	18.384	2642	2646	2653	rBV	22848	29173	5.58%	1.080%
20	19.642	2857	2860	2866	rBV2	7729	9168	1.75%	0.339%
21	20.106	2933	2939	2944	rBV	422311	523174	100.00%	19.369%
22	21.404	3155	3160	3167	rVB2	18232	23749	4.54%	0.879%
23	21.775	3217	3223	3229	rVB	71065	115953	22.16%	4.293%
24	23.502	3512	3517	3523	rVB2	19028	32436	6.20%	1.201%
25	25.059	3774	3782	3795	rVB2	37132	102654	19.62%	3.801%

Sum of corrected areas: 2701035

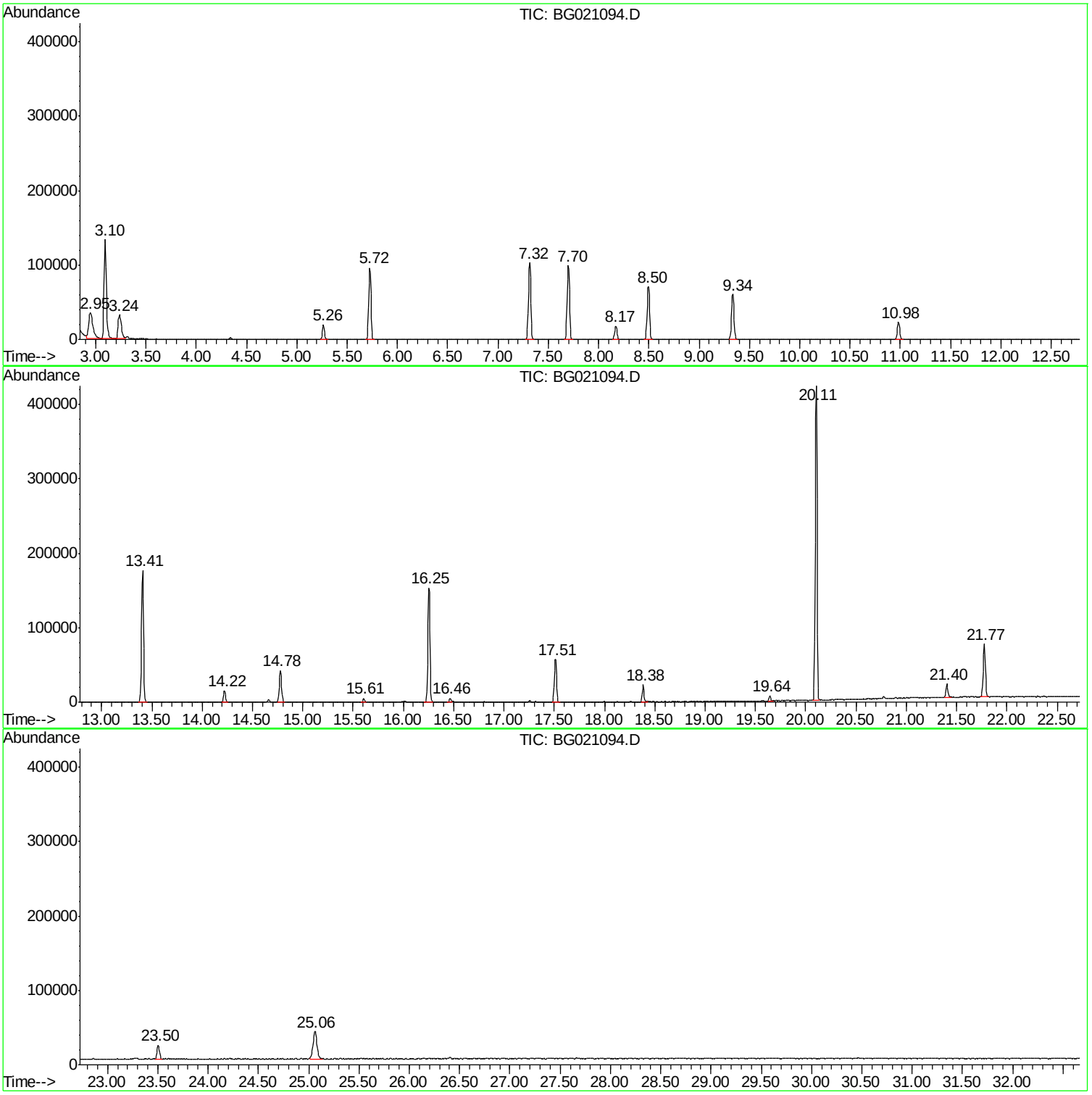
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022616\
Data File : BG021094.D
Acq On : 27 Feb 2016 1:24
Operator : UM/SJ
Sample : H1558-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022616\
Data File : BG021094.D
Acq On : 27 Feb 2016 1:24
Operator : UM/SJ
Sample : H1558-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

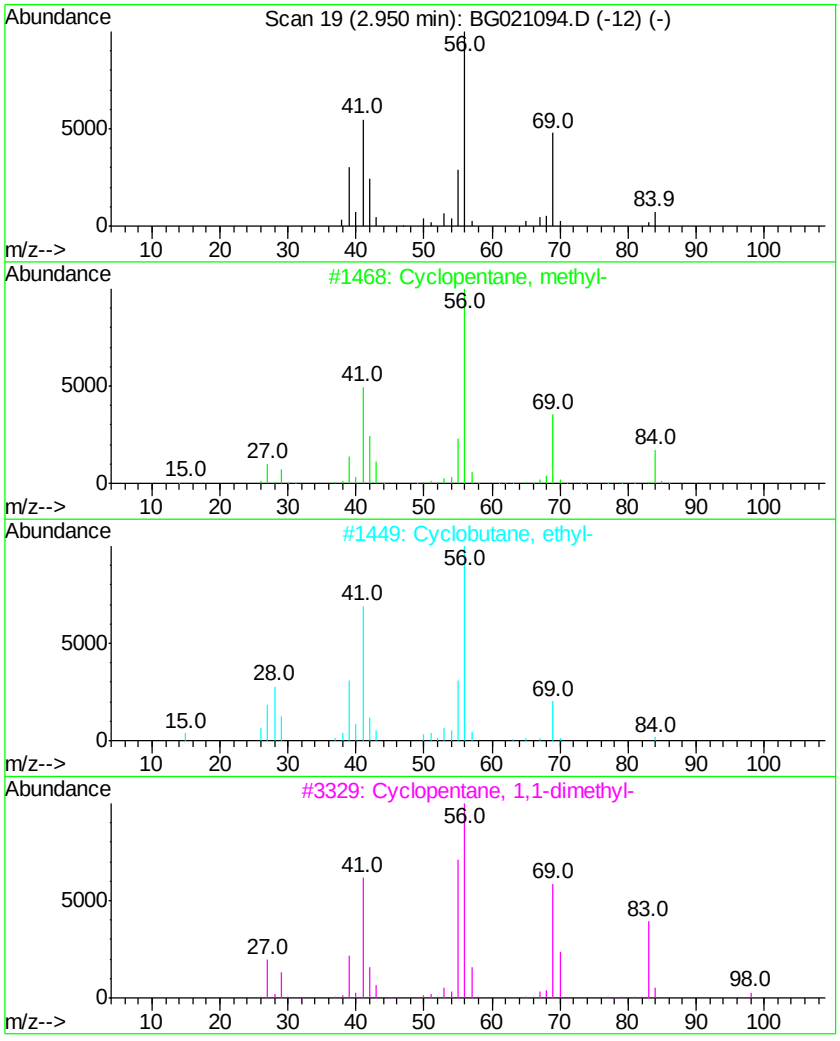
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

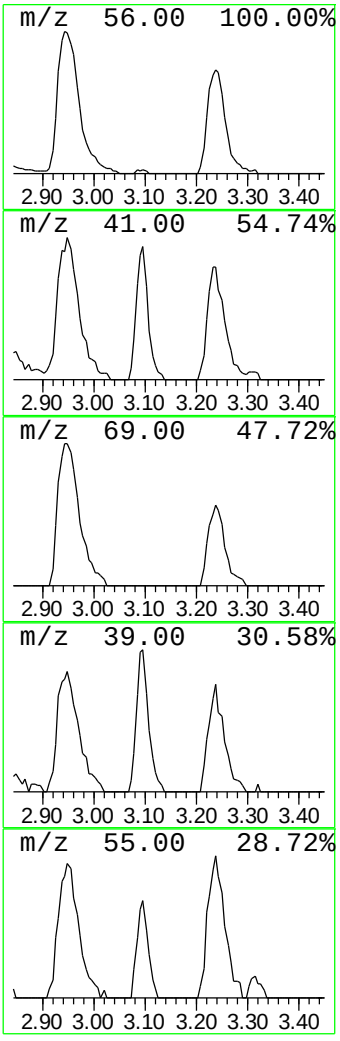
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.95	71.60 ng	103336	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
3	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	39
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	39





Data Path : Z:\HPCHEM1\BNA G\DATA\BG022616\
Data File : BG021094.D
Acq On : 27 Feb 2016 1:24
Operator : UM/SJ
Sample : H1558-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

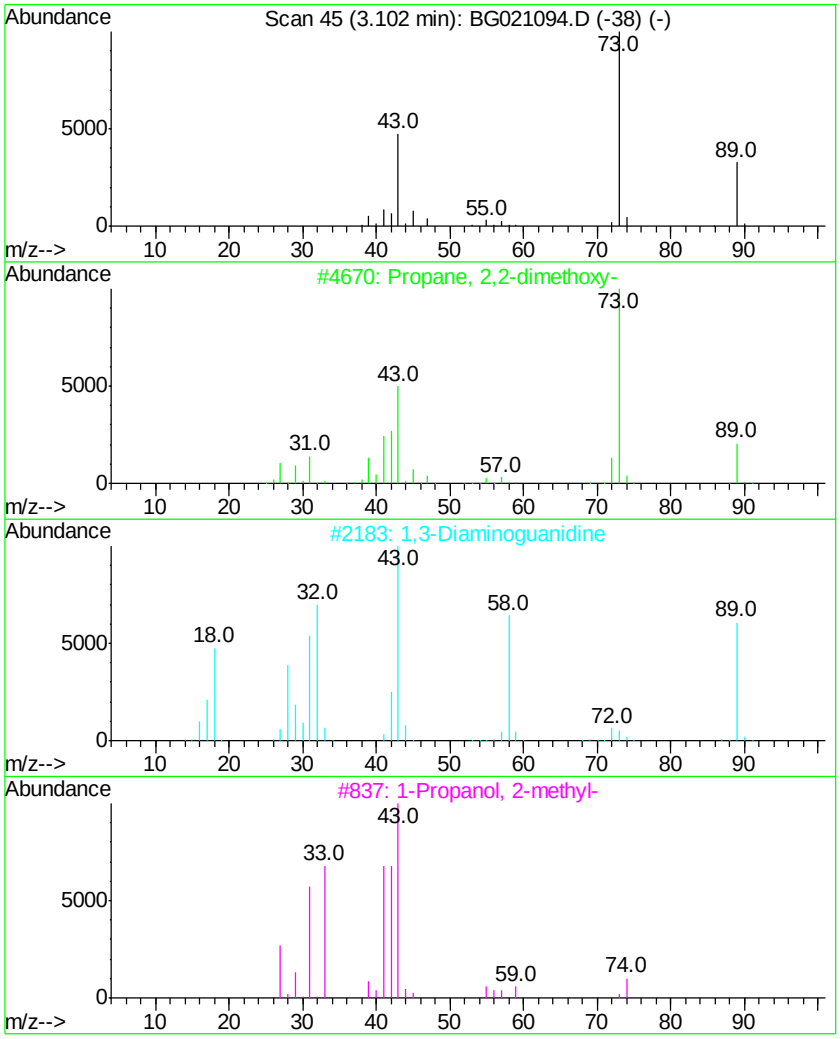
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

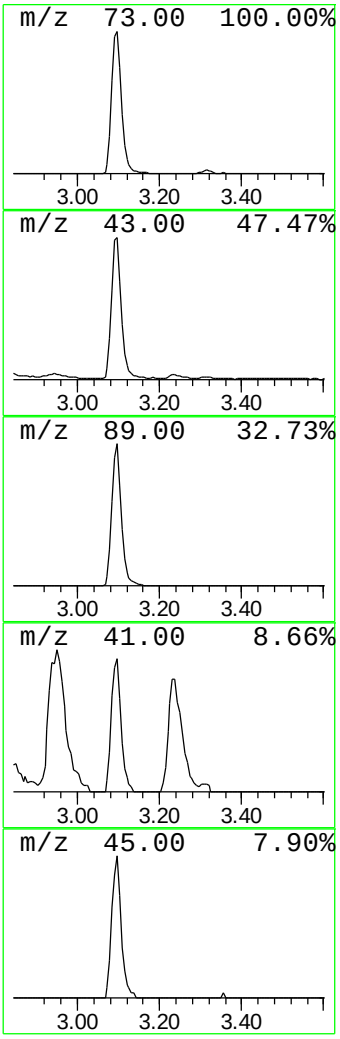
****

Peak Number 2 unknown3.10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.10	146.58 ng	211561	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	Methylglyoxal	72	C3H4O2	000078-98-8	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG022616\
Data File : BG021094.D
Acq On : 27 Feb 2016 1:24
Operator : UM/SJ
Sample : H1558-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

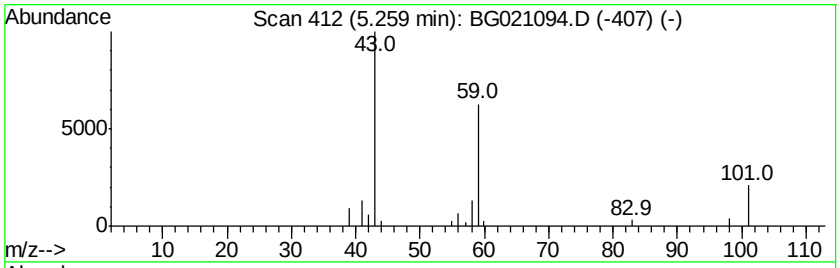
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

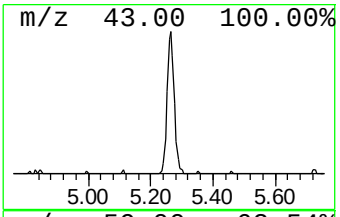
****

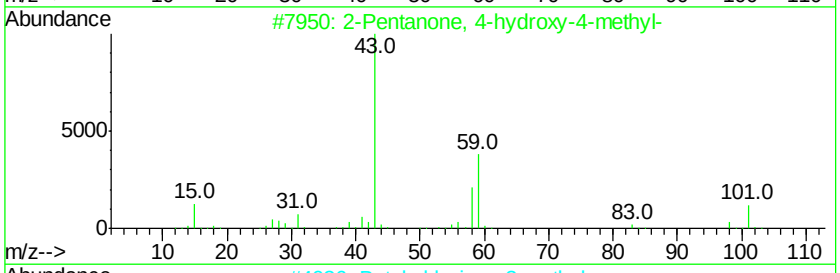
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

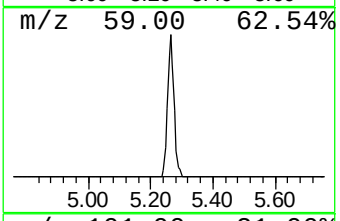
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	20.52 ng	29616	1,4-Dichlorobenzene-d4	8.17

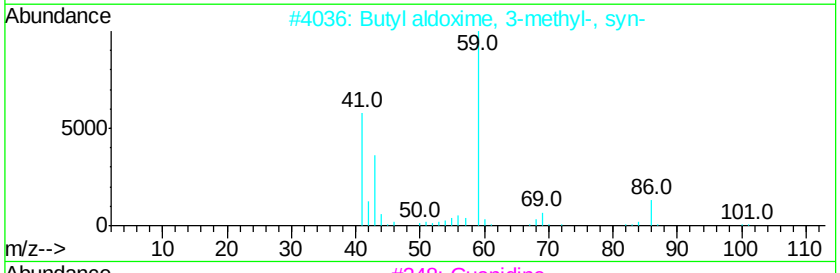
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
3	Guanidine	59	CH5N3	000113-00-8	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9

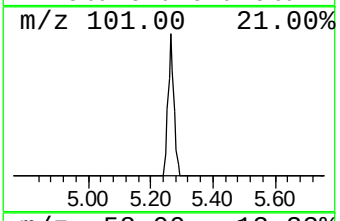


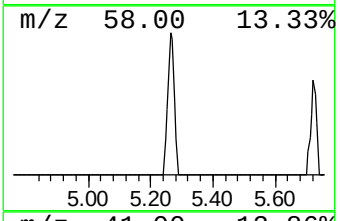


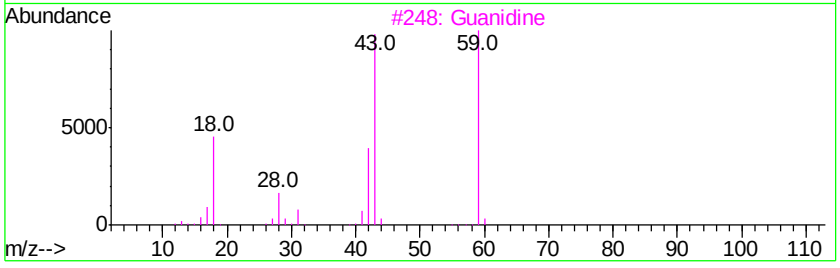


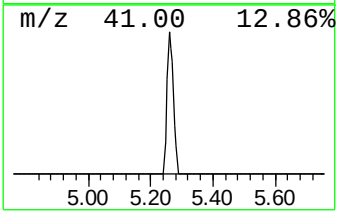












Data Path : Z:\HPCHEM1\BNA G\DATA\BG022616\
Data File : BG021094.D
Acq On : 27 Feb 2016 1:24
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Sample : H1558-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

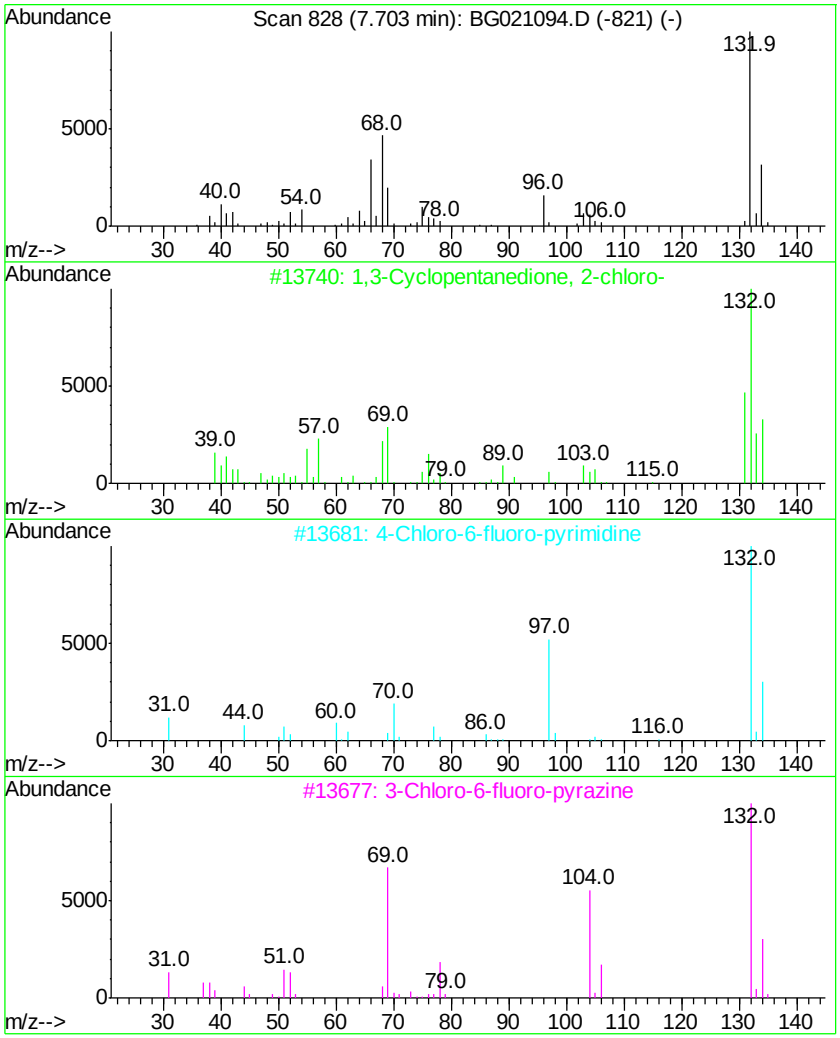
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

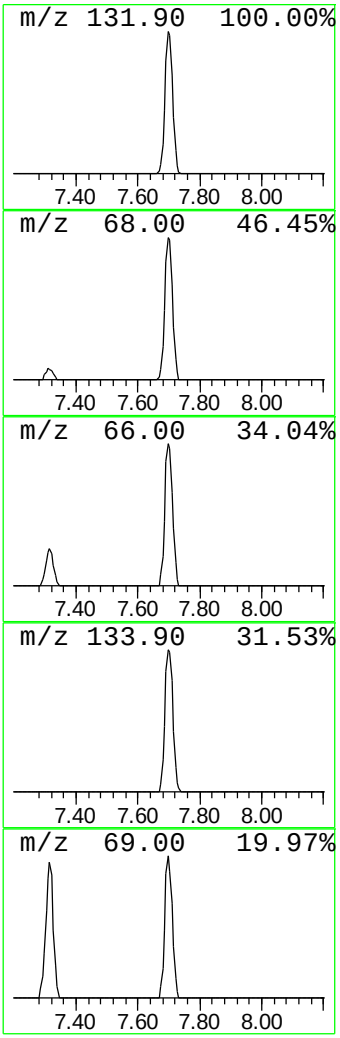
****

Peak Number 5 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	114.89 ng	165822	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	32
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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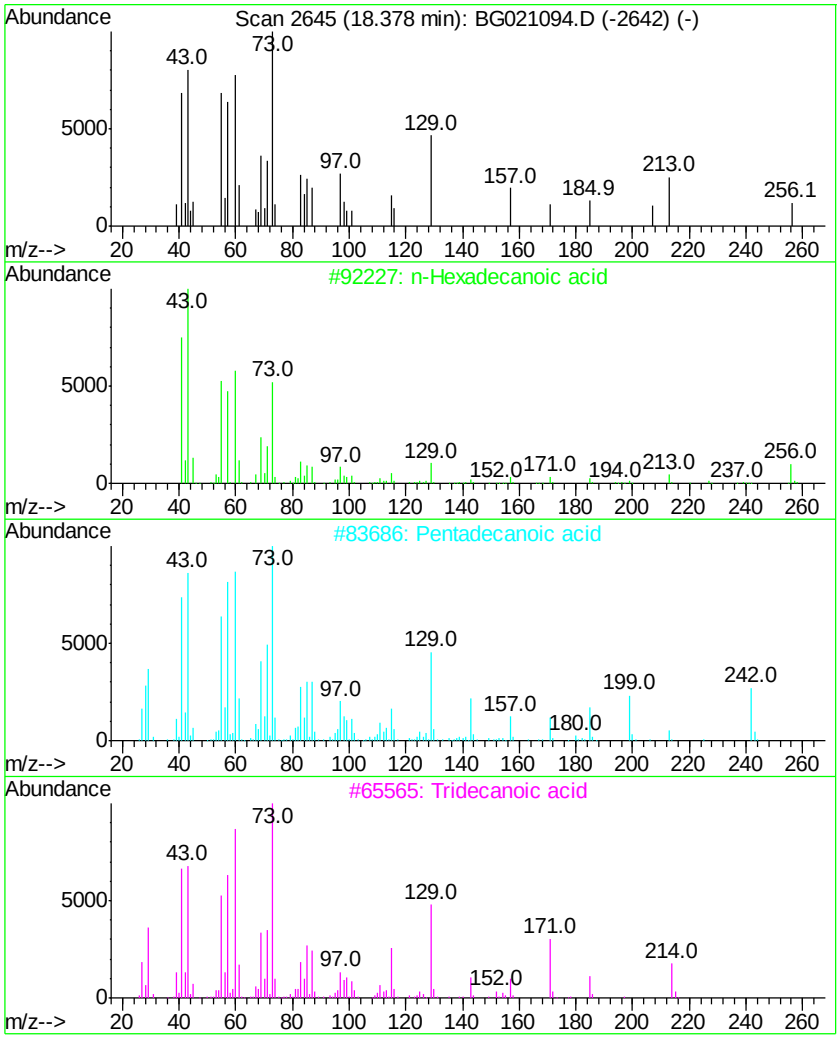
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

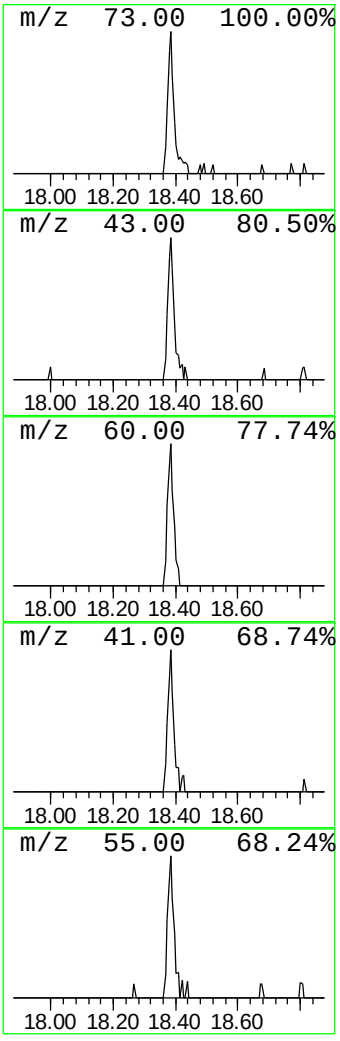
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	6.78 ng	29173	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Operator : UM/SJ
Sample : H1558-07
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Instrument : BNA_G
ClientSampleId : S9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

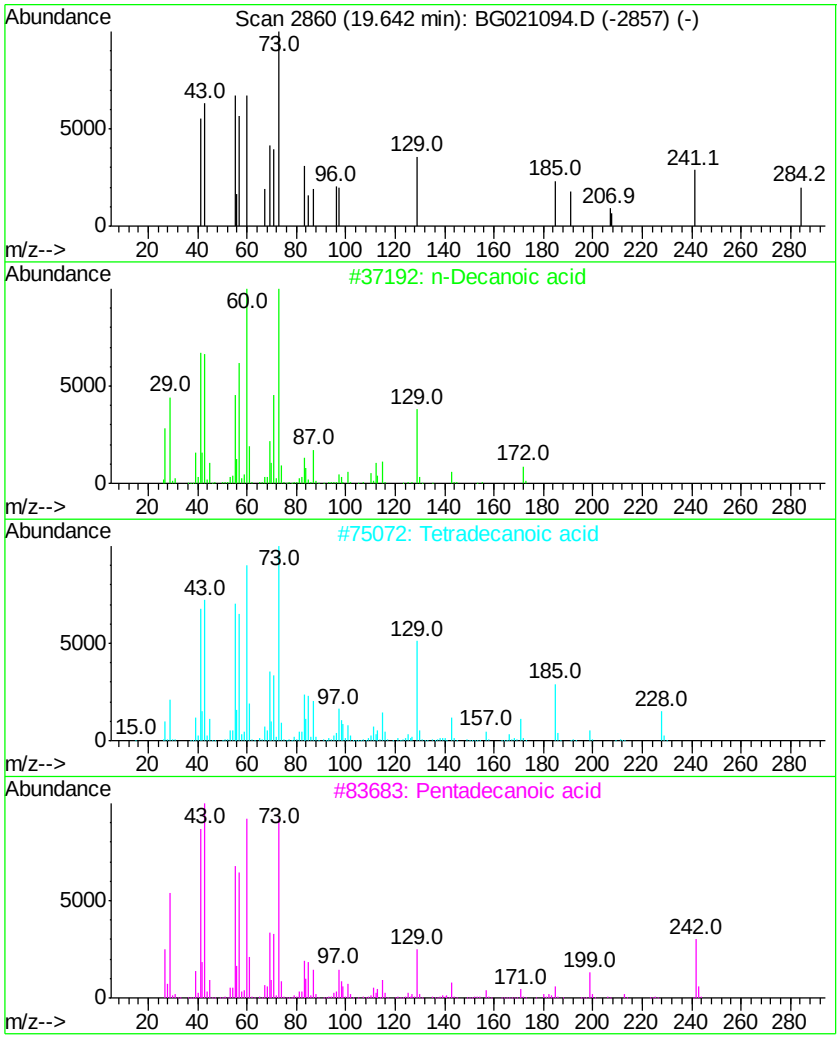
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

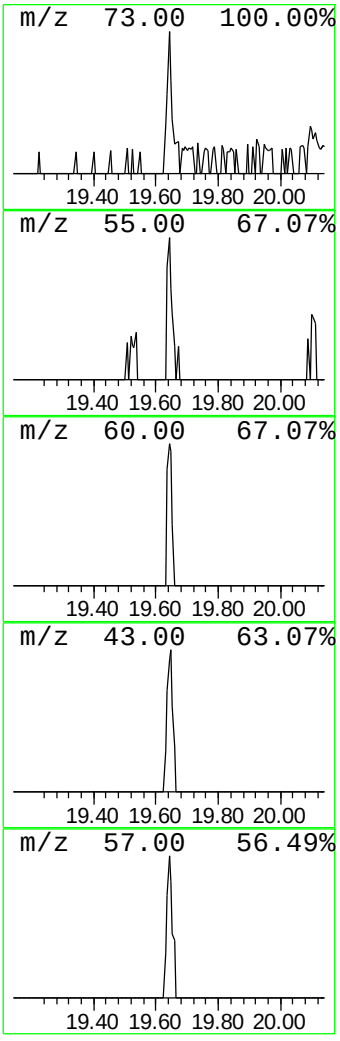
****

Peak Number 8 unknown19.64 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.64	2.13 ng	9168	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	43
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	37
4	Lactose	342	C12H22O11	000063-42-3	17
5	.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	17





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ClientSampleId : S9

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

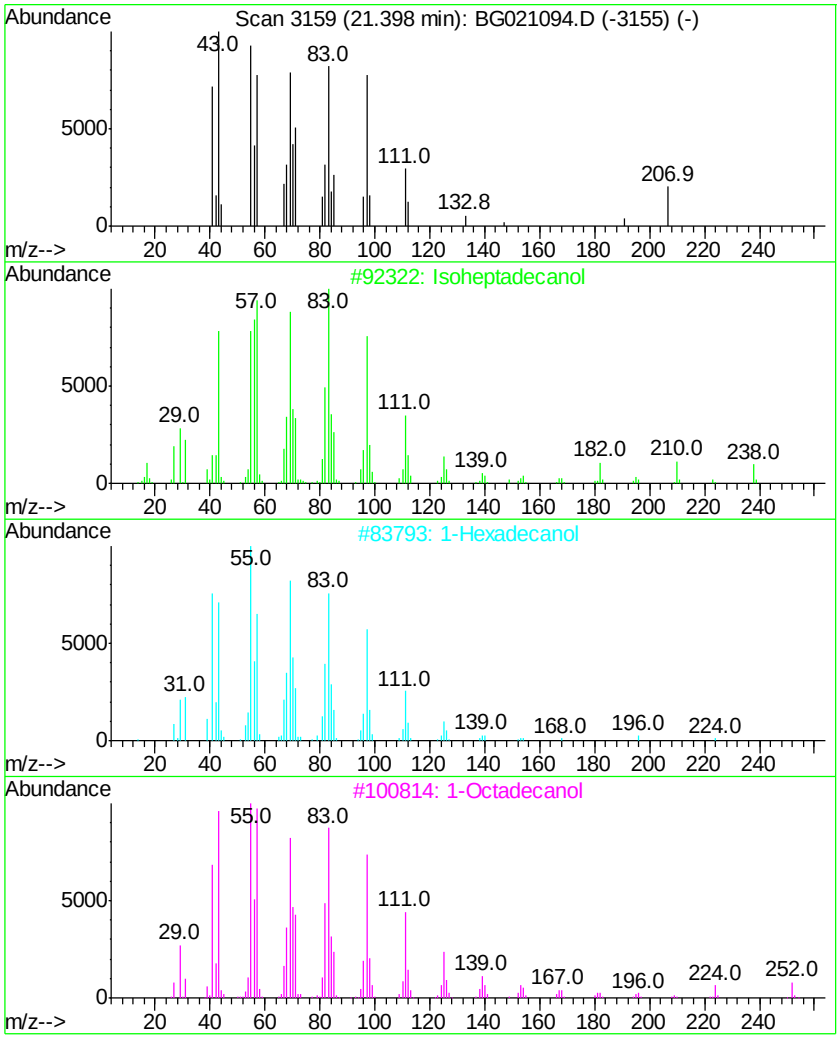
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

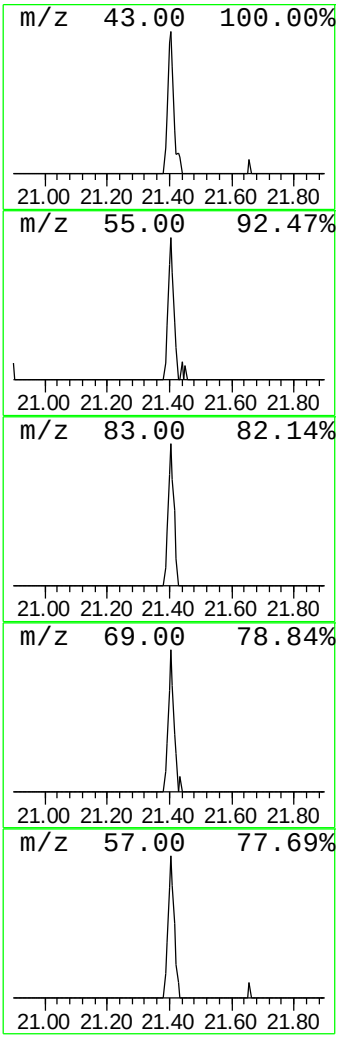
****

Peak Number 9 Isoheptadecanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	4.10 ng	23749	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoheptadecanol	256	C17H36O	057289-07-3	90
2	1-Hexadecanol	242	C16H34O	036653-82-4	90
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
5	1-Heptadecanol	256	C17H36O	001454-85-9	81





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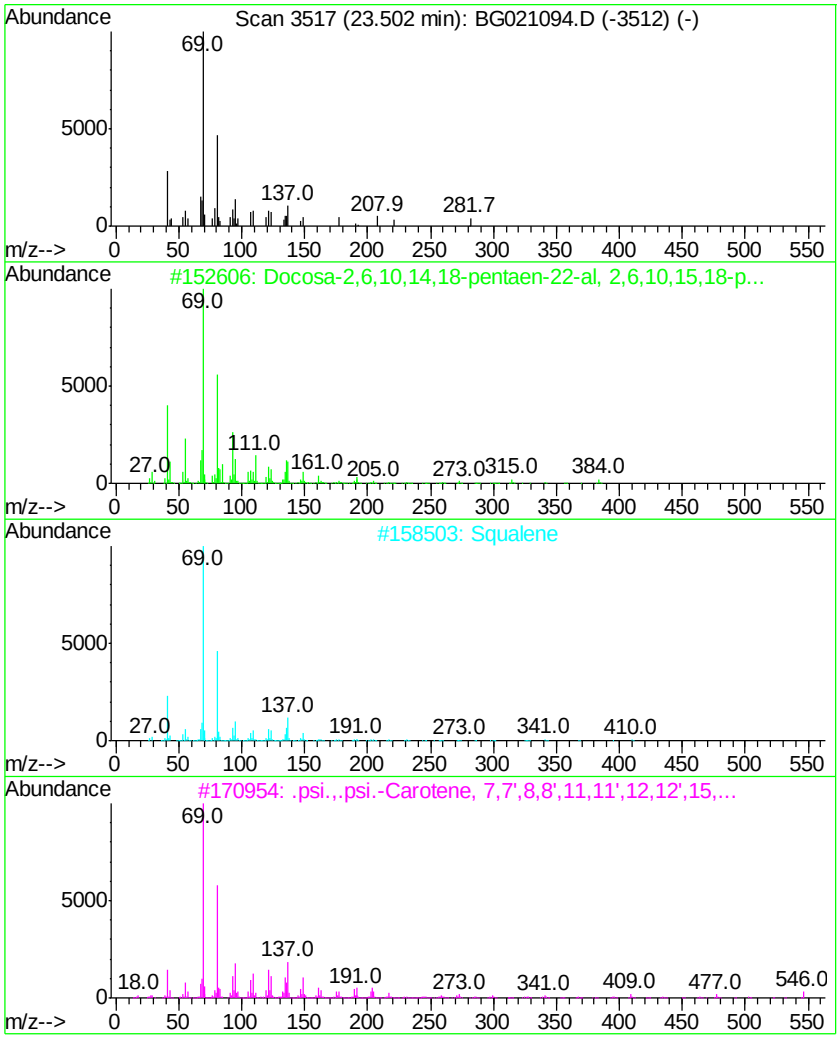
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

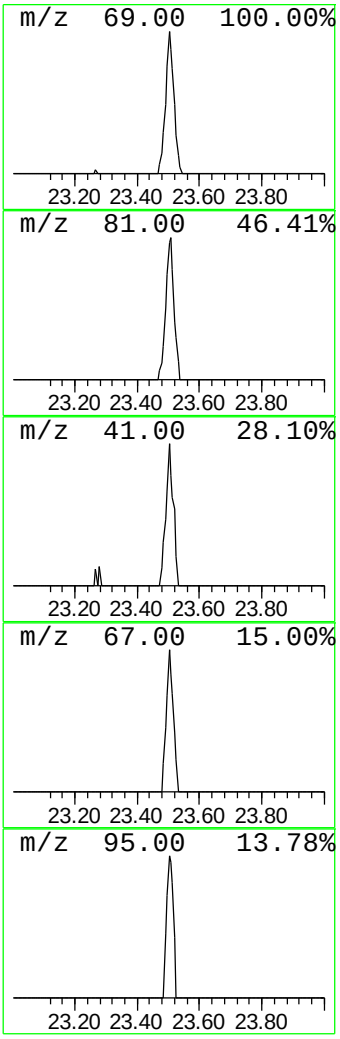
****

Peak Number 10 Docosa-2,6,10,14,18-pentaen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.50	6.32 ng	32436	Perylene-d12	25.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
2	Squalene	410	C30H50	007683-64-9	80
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG022616\
Data File : BG021094.D
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, met...	2.95	71.6	ng	103336	1	8.17	28866	20.0
unknown3.10	3.10	146.6	ng	211561	1	8.17	28866	20.0
2-Pentanone, 4-hy...	5.26	20.5	ng	29616	1	8.17	28866	20.0
unknown7.70	7.70	114.9	ng	165822	1	8.17	28866	20.0
n-Hexadecanoic acid	18.38	6.8	ng	29173	4	17.51	86090	20.0
unknown19.64	19.64	2.1	ng	9168	4	17.51	86090	20.0
Isoheptadecanol	21.40	4.1	ng	23749	5	21.77	115953	20.0
Docosa-2,6,10,14,...	23.50	6.3	ng	32436	6	25.07	102654	20.0