LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023137.D
Acq On : 16 Jul 2016 8:17
Operator : UM/SJ
Sample : H4015-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-20

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-BG070816.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	2.896	5	10	25	rVB2	208075	505266	5.49%	0.837%
2	3.037	29	34	53	rVV	5855105	9208270	100.00%	15.262%
3	3.184	55	59	76	rVV	177467	382116	4.15%	0.633%
4	5.217	399	405	412	rVB	265194	416250	4.52%	0.690%
5	5.698	479	487	498	rBV	2008260	3333802	36.20%	5.525%
6	7.308	753	761	773	rBV	2286364	4108466	44.62%	6.809%
7	7.678	817	824	829	rBV	2151280	3747409	40.70%	6.211%
8	7.725	829	832	847	rVB	333227	529297	5.75%	0.877%
9	8.148	896	904	912	rVB	401901	689485	7.49%	1.143%
10	8.478	952	960	968	rVB	1466342	2553523	27.73%	4.232%
11	9.324	1096	1104	1112	rBV	1478726	2602192	28.26%	4.313%
12	10.980	1379	1386	1394	rBV	606984	1122908	12.19%	1.861%
13	13.419	1792	1801	1813	rBV	3712113	6045505	65.65%	10.020%
14	14.241	1933	1941	1947	rBV	846738	1234224	13.40%	2.046%
15	14.800	2029	2036	2044	rBV2	1088028	1787999	19.42%	2.963%
16	16.292	2283	2290	2300	rBV	3455065	5368696	58.30%	8.898%
17	16.480	2318	2322	2330	rBV2	71988	119294	1.30%	0.198%
18	17.273	2454	2457	2462	rBV	82740	103938	1.13%	0.172%
19	17.555	2498	2505	2517	rBV2	1327306	2251497	24.45%	3.732%
20	18.419	2647	2652	2657	rBV2	221492	318491	3.46%	0.528%
21	20.152	2940	2947	2955	rBV	6128629	8176416	88.79%	13.551%
22	21.474	3167	3172	3173	rBV4	76142	111663	1.21%	0.185%
23	21.850	3229	3236	3243	rBV	1464320	2519192	27.36%	4.175%
24	23.577	3523	3530	3537	rBV	400618	772103	8.38%	1.280%
25	25.223	3799	3810	3822	rBV2	727072	2328419	25.29%	3.859%

Sum of corrected areas: 60336421

LSC Report - Integrated Chromatogram

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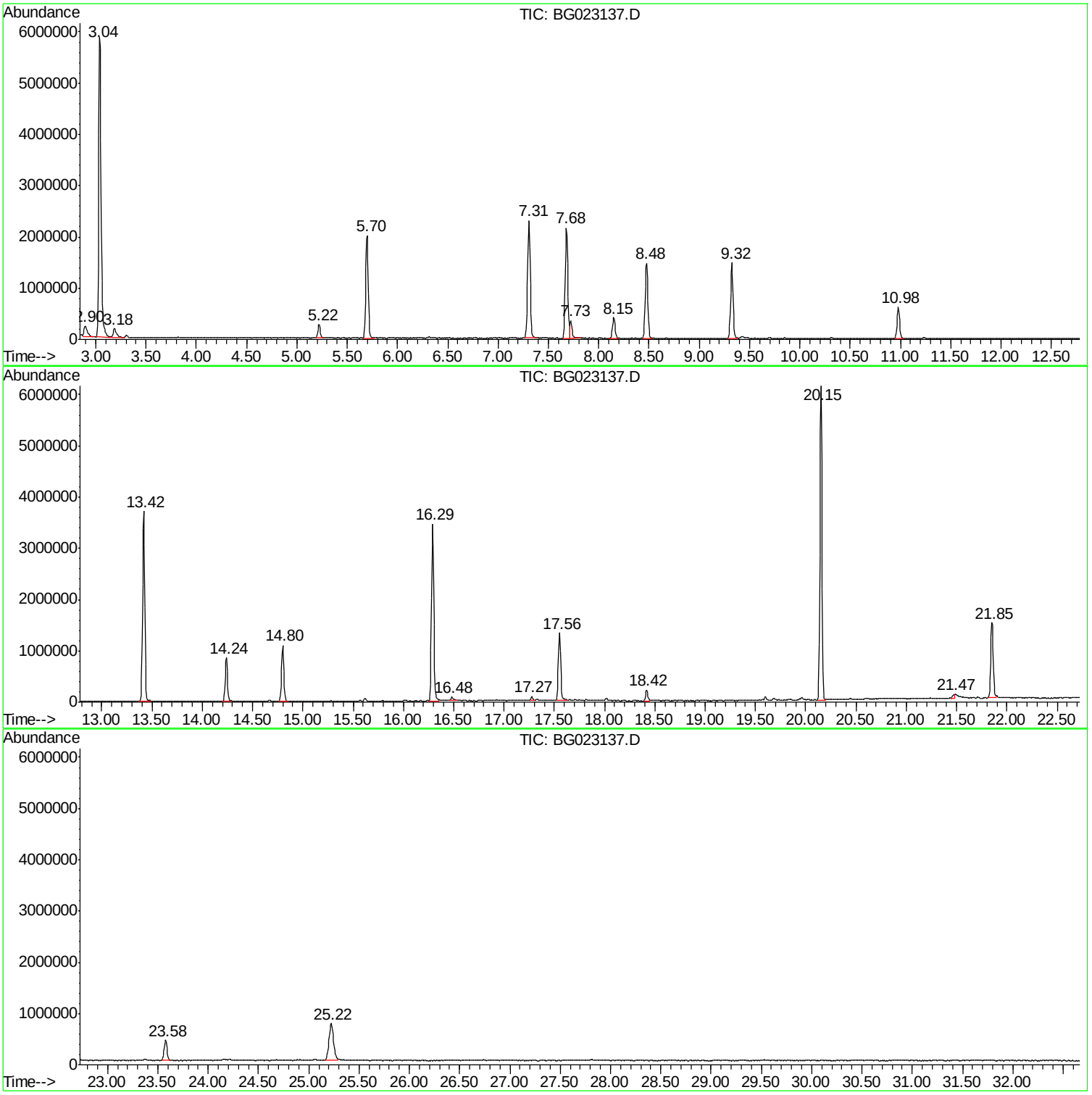
Operator : UM/SJ
Sample : H4015-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023137.D
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Operator : UM/SJ
Sample : H4015-19
Misc :
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Instrument : BNA_G
ClientSampleId : C5-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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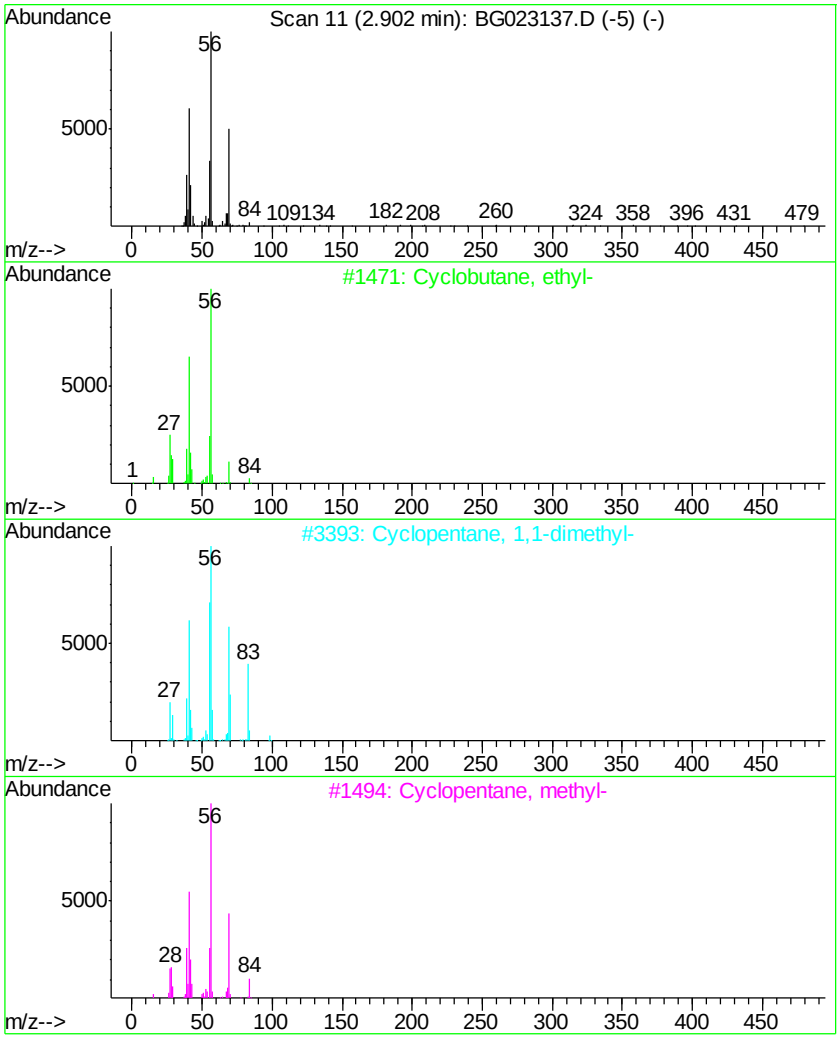
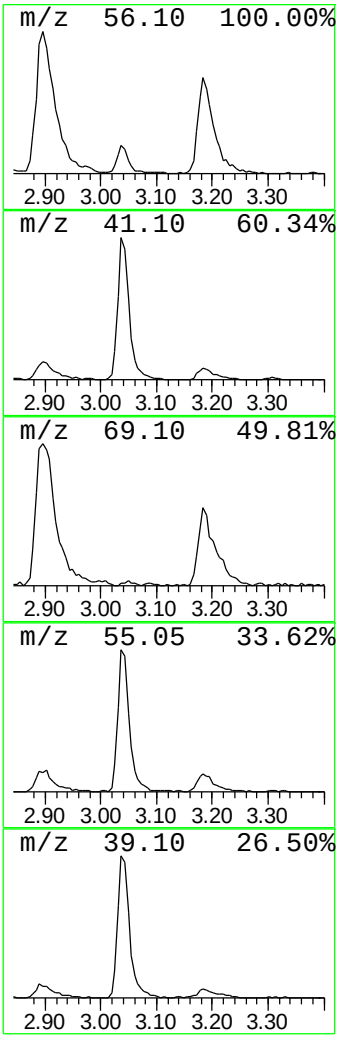
Peak Number 1 Cyclobutane, ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	14.66 ng	505266	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
2	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	72
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	45
5	2-Oxepanone, 4-methyl-	128	C7H12O2	002549-60-2	40





Library Search Compound Report

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Data File : BG023137.D
Acq On : 16 Jul 2016 8:17
Operator : UM/SJ
Sample : H4015-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

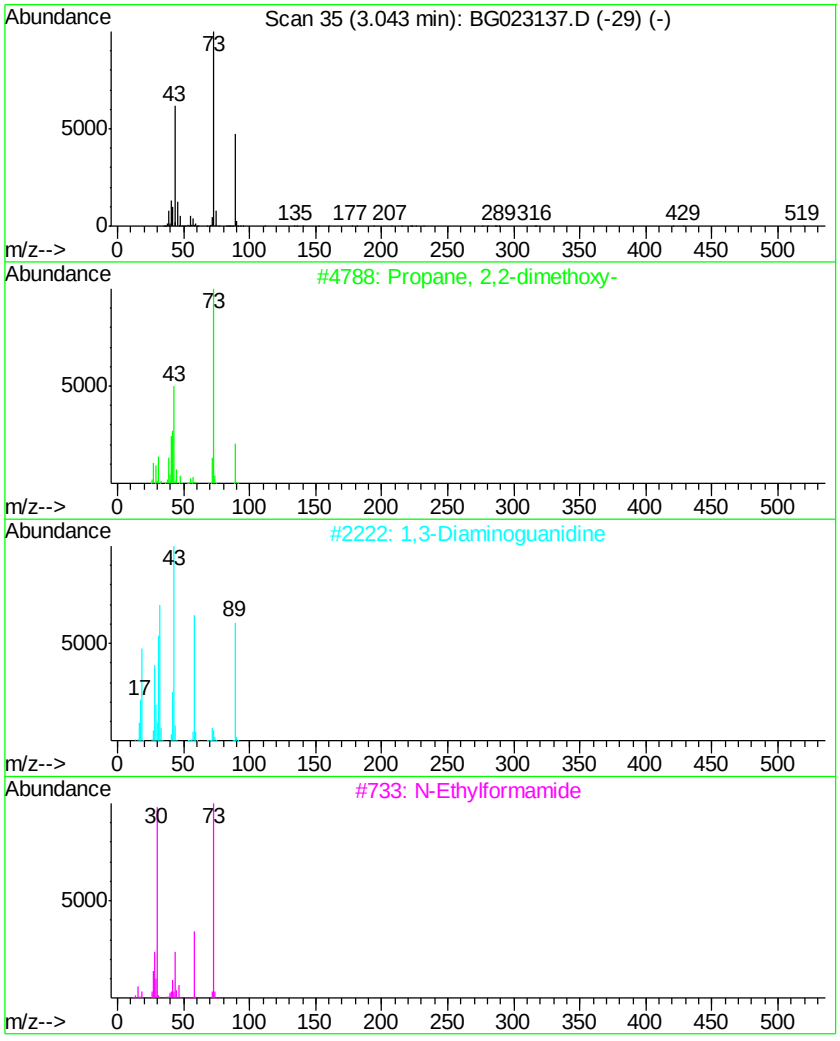
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

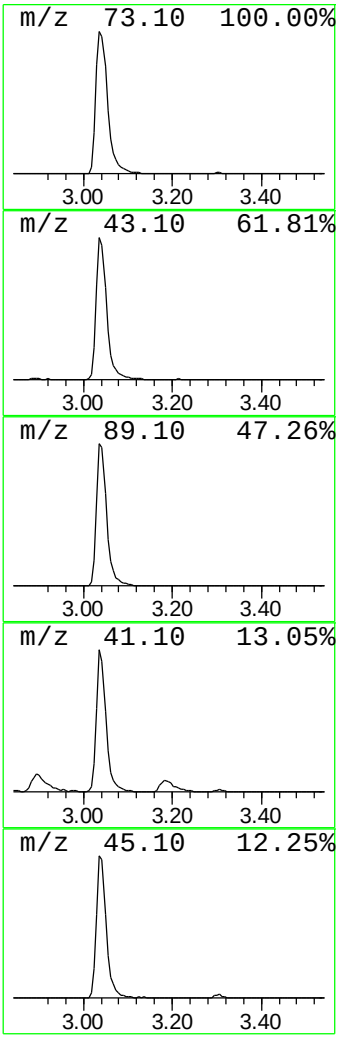
****

Peak Number 2 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	267.11 ng	9208270	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	40
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	23
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





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Data File : BG023137.D
Acq On : 16 Jul 2016 8:17
Operator : UM/SJ
Sample : H4015-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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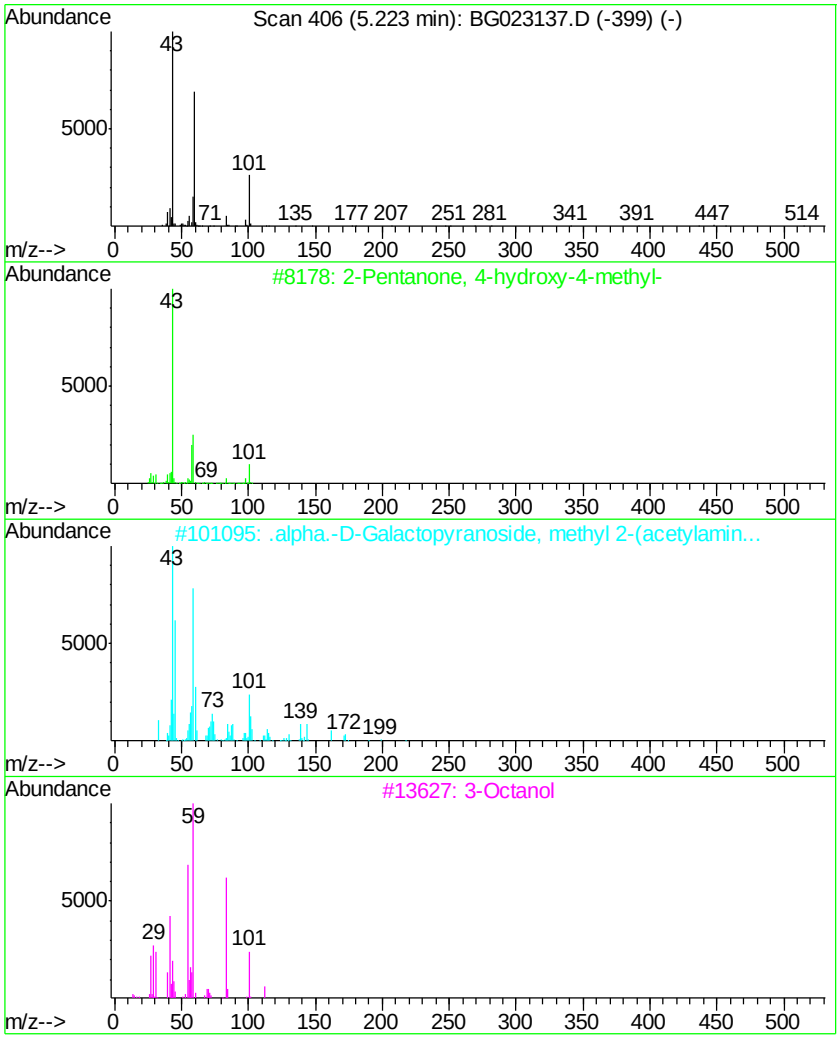
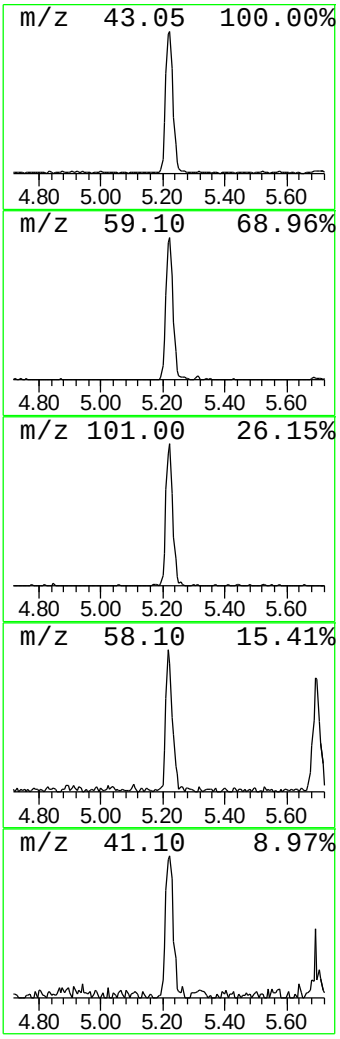
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	12.07 ng	416250	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	39
3	3-Octanol	130	C8H18O	000589-98-0	33
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	27
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12





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Acq On : 16 Jul 2016 8:17
Operator : UM/SJ
Sample : H4015-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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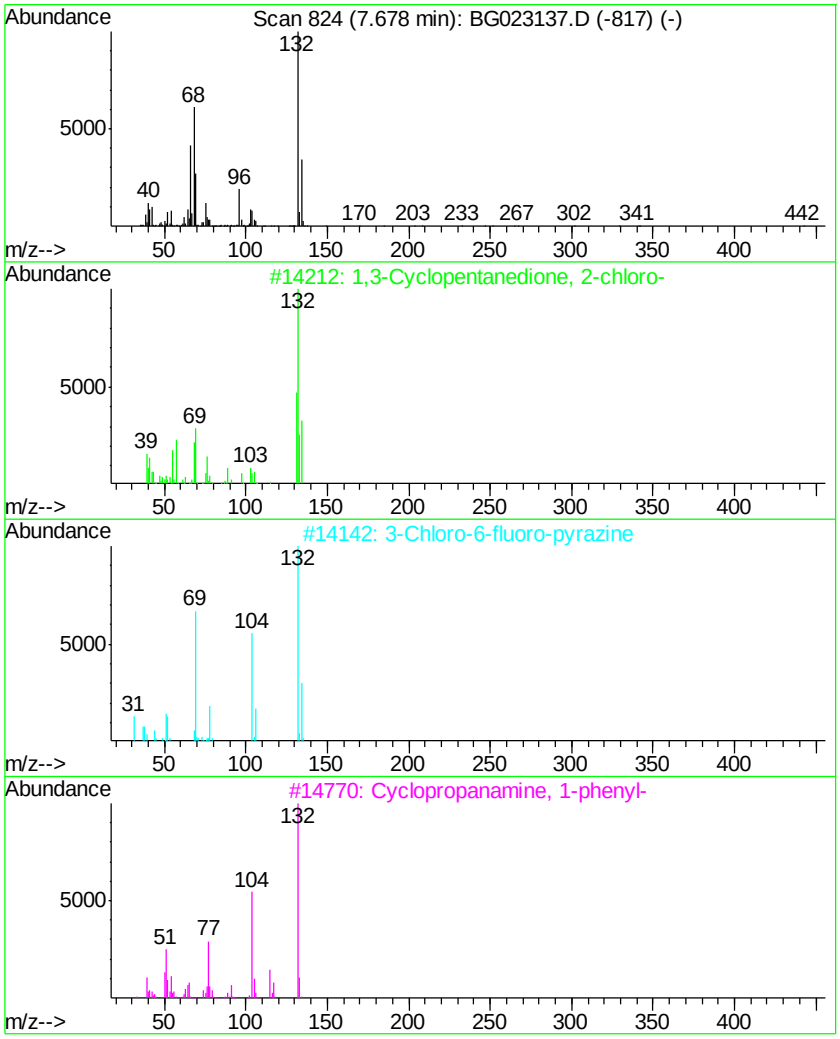
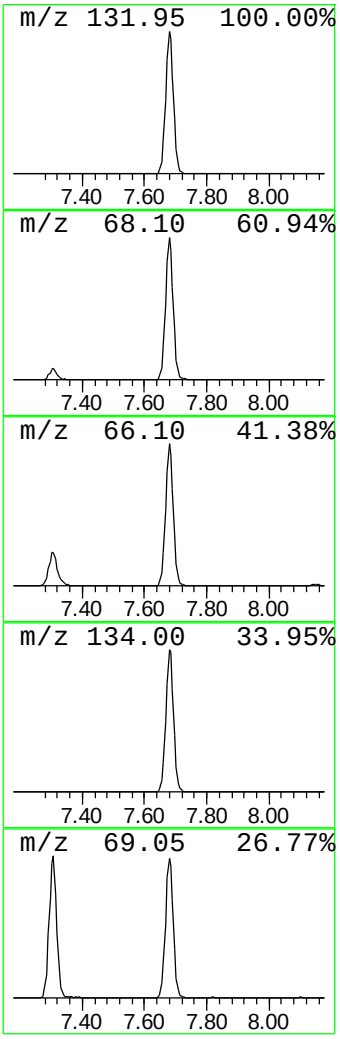
Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	108.70 ng	3747410	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10





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Operator : UM/SJ
Sample : H4015-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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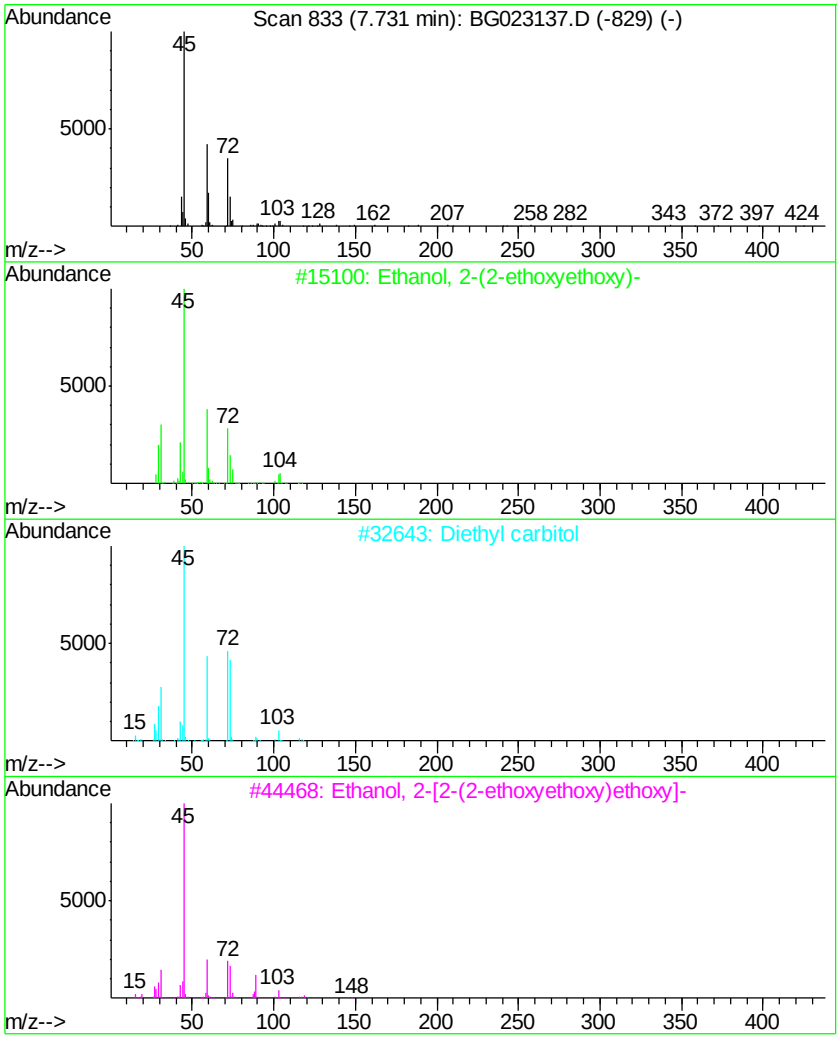
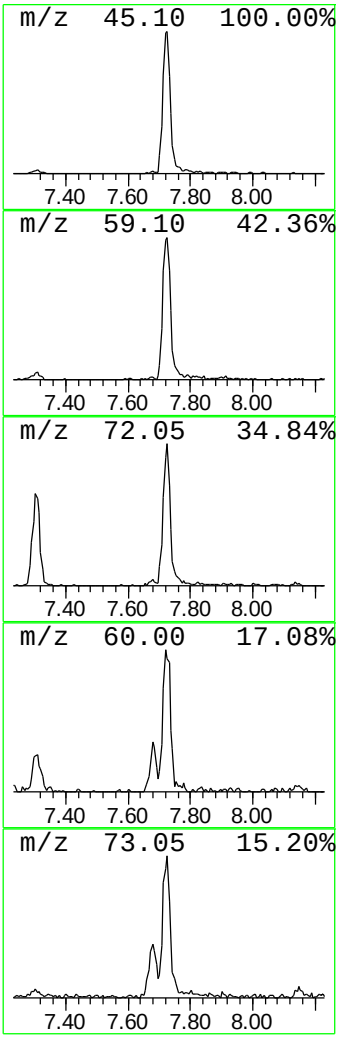
Peak Number 6 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	15.35 ng	529297	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	64
2	Diethyl carbitol	162	C8H18O3	000112-36-7	50
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5	.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	36





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Sample : H4015-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

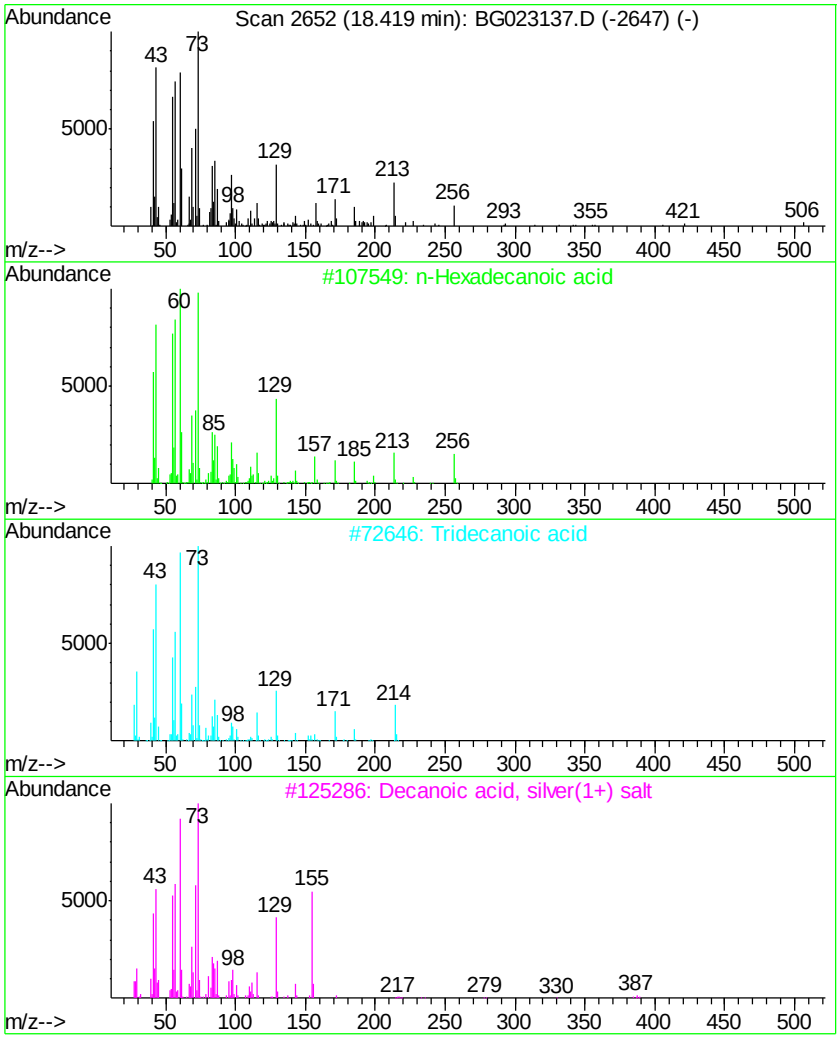
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

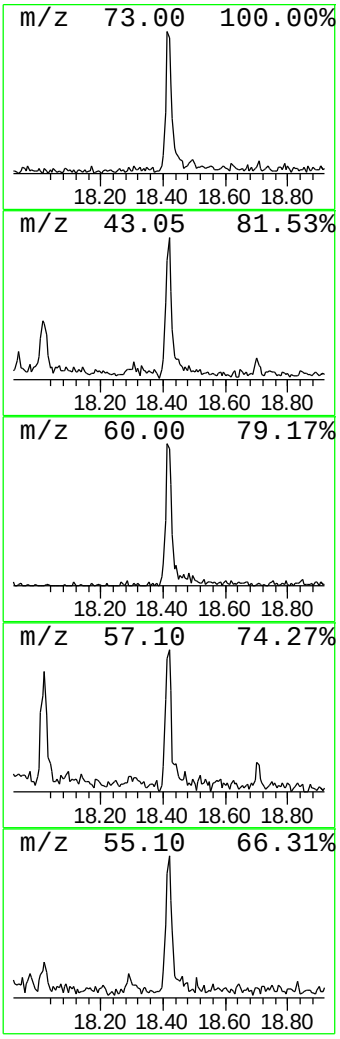
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.83 ng	318491	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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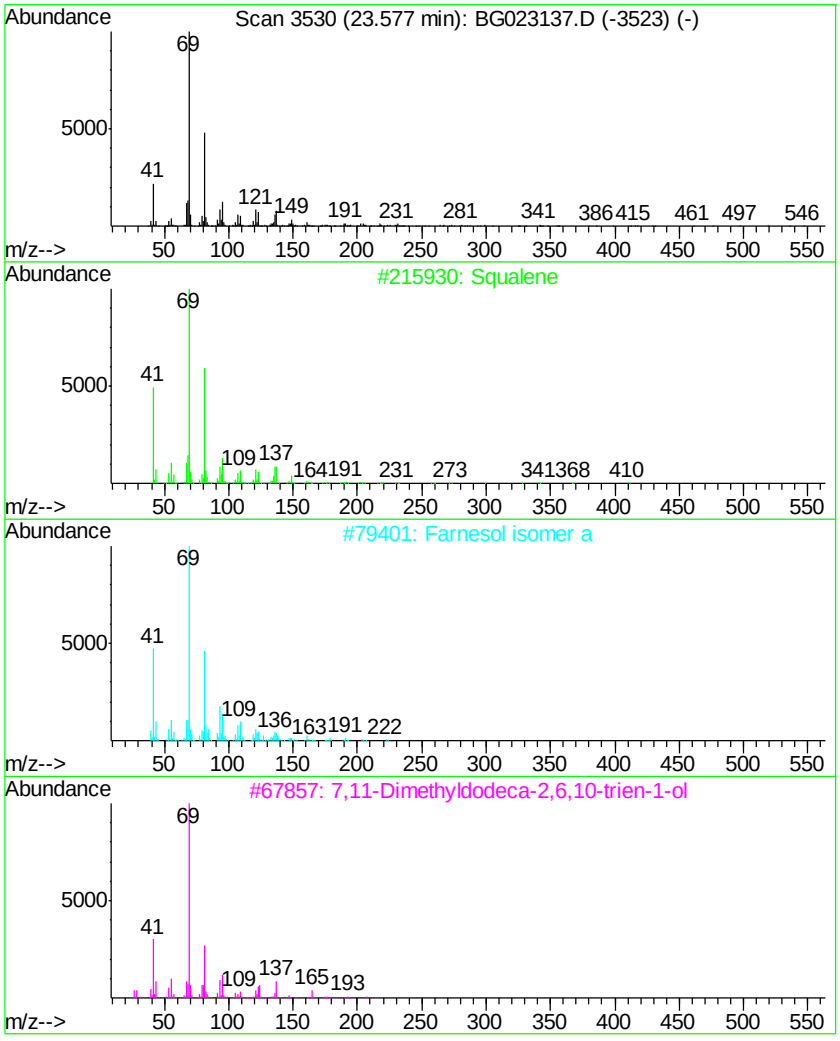
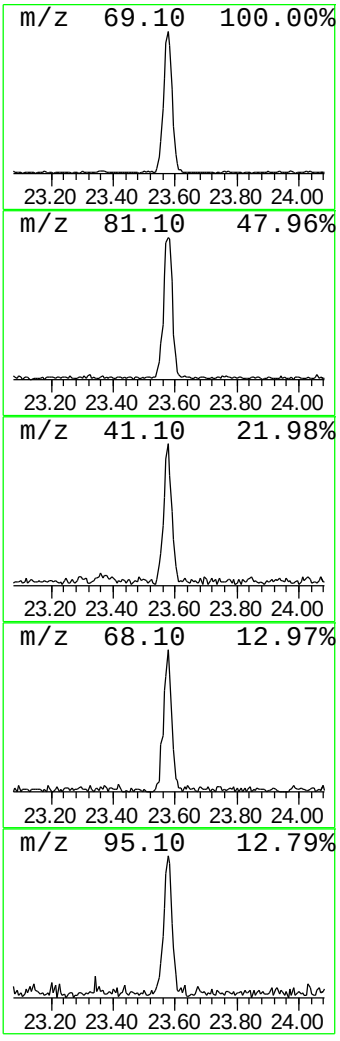
Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	6.63 ng	772103	Perylene-d12	25.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Farnesol isomer a	222	C15H26O	1000108-92-4	72
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	59





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclobutane, ethyl-	2.90	14.7	ng	505266	1	8.15	689485	20.0
unknown3.04	3.04	267.1	ng	9208270	1	8.15	689485	20.0
2-Pentanone, 4-hy...	5.22	12.1	ng	416250	1	8.15	689485	20.0
unknown7.68	7.68	108.7	ng	3747410	1	8.15	689485	20.0
Ethanol, 2-(2-eth...	7.73	15.4	ng	529297	1	8.15	689485	20.0
n-Hexadecanoic acid	18.42	2.8	ng	318491	4	17.56	2251500	20.0
Squalene	23.58	6.6	ng	772103	6	25.22	2328420	20.0