LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024618.D
Acq On : 2 Nov 2016 8:18
Operator : UM/SJ
Sample : H5489-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-70-11.5-12.0

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-BG102516.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	2.978	18	24	44	rVB	7052023	22897838	100.00%	20.996%
2	3.125	44	49	67	rVB	7861884	16244026	70.94%	14.895%
3	3.272	67	74	101	rVB	5264454	14545625	63.52%	13.338%
4	3.537	114	119	130	rVB2	121646	244728	1.07%	0.224%
5	5.329	418	424	433	rVB	536383	871336	3.81%	0.799%
6	5.799	496	504	514	rBV	2414936	4065948	17.76%	3.728%
7	7.403	766	777	790	rBV	2456230	4434394	19.37%	4.066%
8	7.796	835	844	856	rVB	2340075	4222111	18.44%	3.871%
9	8.266	916	924	931	rBV2	477399	858003	3.75%	0.787%
10	8.595	971	980	992	rBV	1771907	3260301	14.24%	2.990%
11	9.441	1114	1124	1133	rBV	1473412	2817416	12.30%	2.583%
12	11.092	1397	1405	1413	rBV	609290	1118995	4.89%	1.026%
13	13.507	1806	1816	1825	rBV	3992273	6254466	27.31%	5.735%
14	14.318	1947	1954	1962	rBV	746088	1148210	5.01%	1.053%
15	14.882	2043	2050	2057	rBV	985689	1576658	6.89%	1.446%
16	16.363	2296	2302	2312	rBV	3368727	5511511	24.07%	5.054%
17	17.626	2510	2517	2523	rBV	1235021	2008470	8.77%	1.842%
18	18.472	2656	2661	2671	rBV2	151520	254067	1.11%	0.233%
19	20.205	2950	2956	2964	rBV	7529127	10078611	44.02%	9.242%
20	21.498	3171	3176	3190	rBV2	268851	538095	2.35%	0.493%
21	21.915	3240	3247	3258	rVB	1605072	2810632	12.27%	2.577%
22	23.642	3534	3541	3551	rVB2	202674	428102	1.87%	0.393%
23	25.346	3816	3831	3843	rBV3	886817	2868405	12.53%	2.630%

Sum of corrected areas: 109057948

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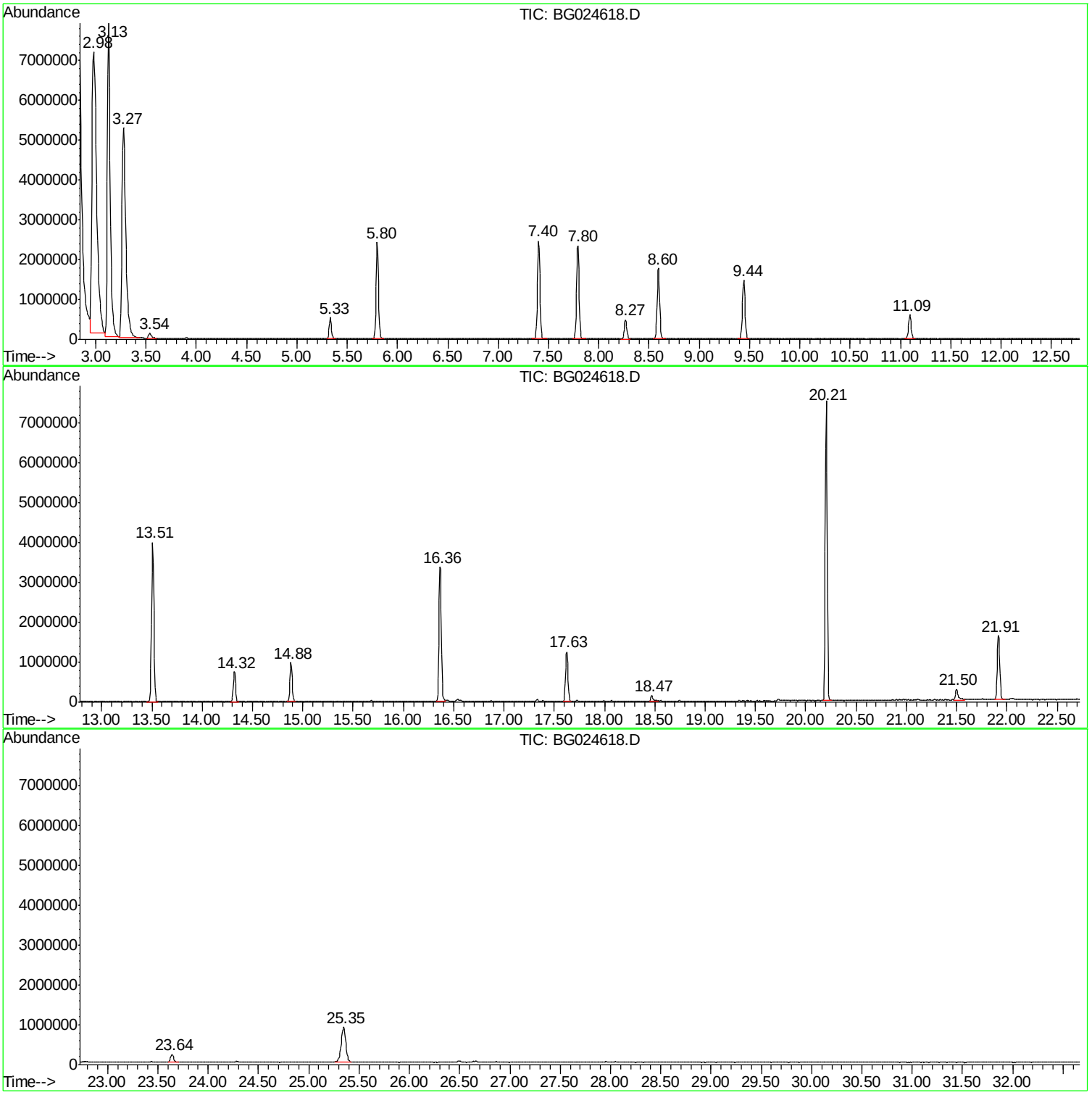
Instrument :
BNA_G
ClientSampleId :
SB-70-11.5-12.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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Acq On : 2 Nov 2016 8:18
Operator : UM/SJ
Sample : H5489-06
Misc :
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

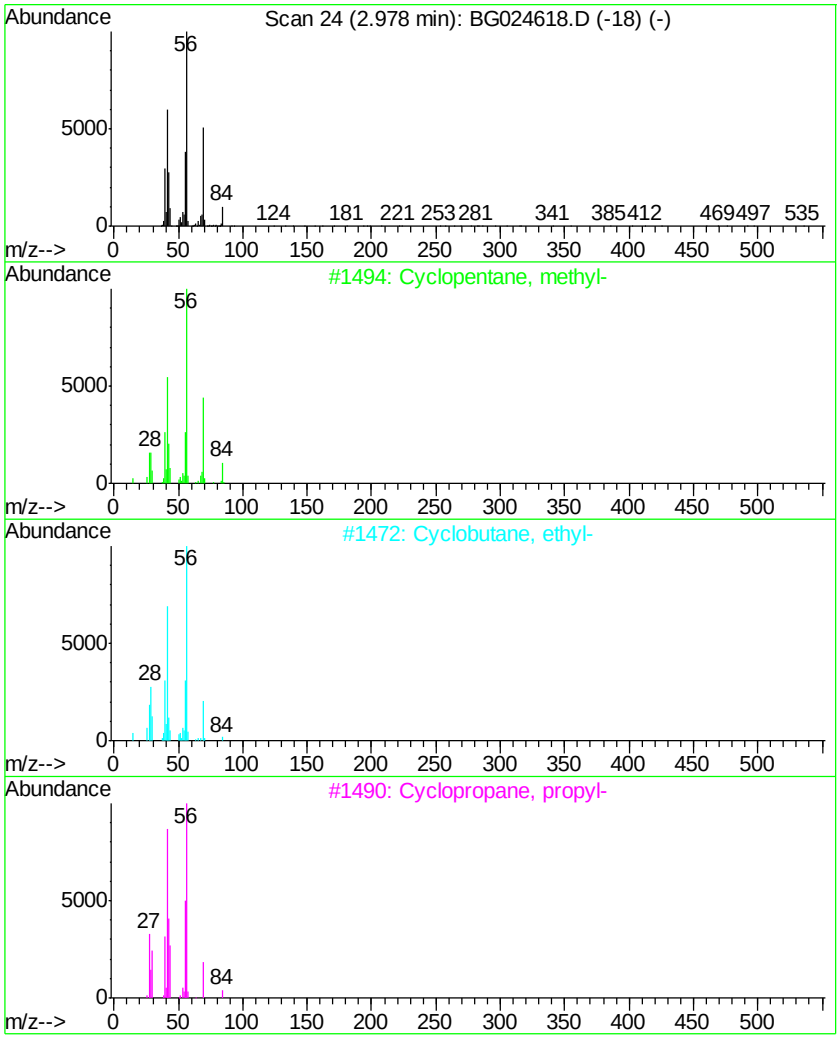
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

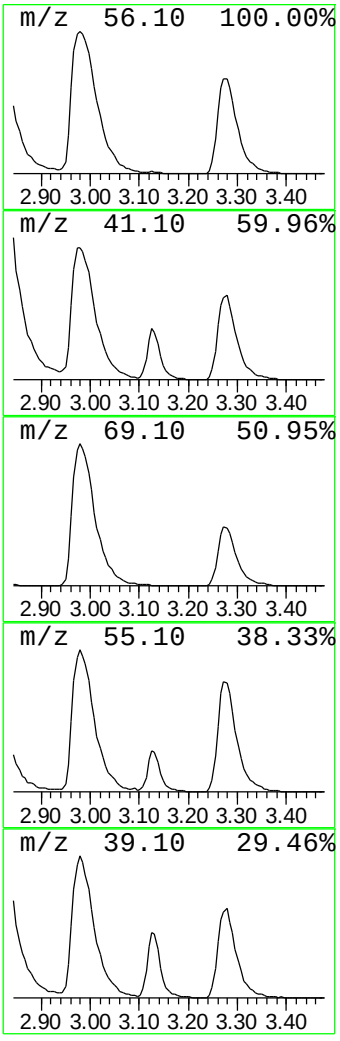
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	533.75 ng	22897800	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
3	Cyclopropane, propyl-	84	C6H12	002415-72-7	50
4	Cyclobutane	56	C4H8	000287-23-0	50
5	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	50





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Operator : UM/SJ
Sample : H5489-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-70-11.5-12.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

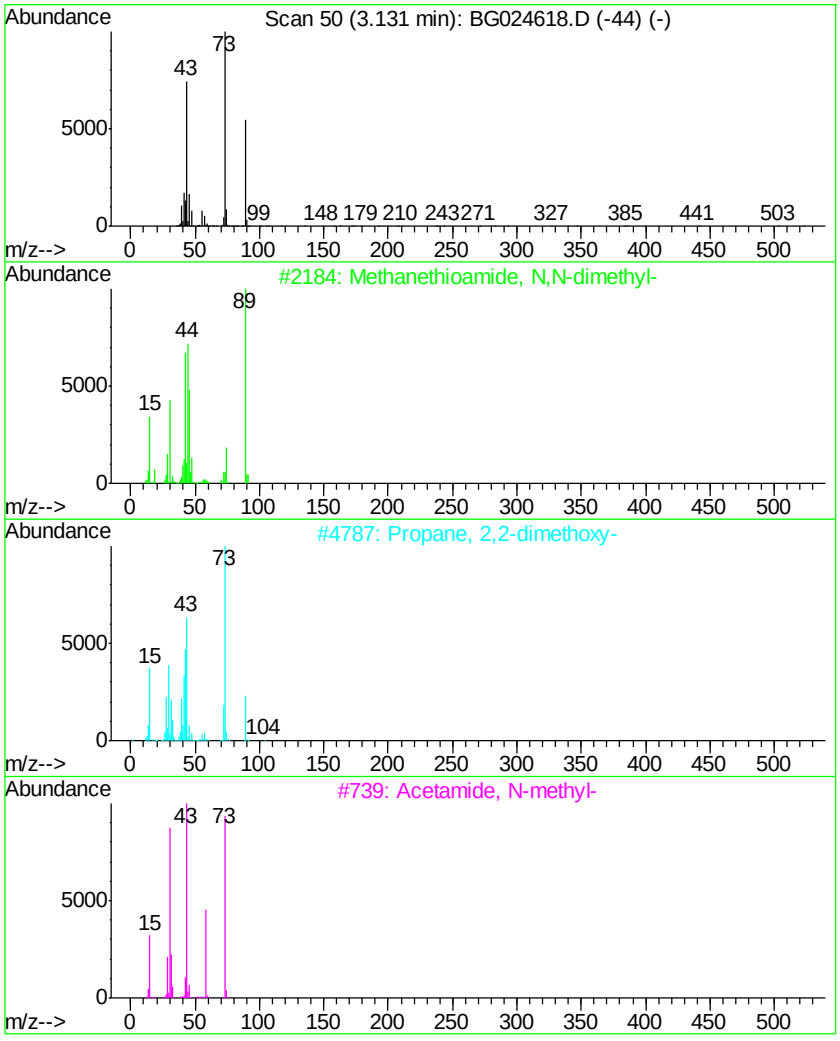
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

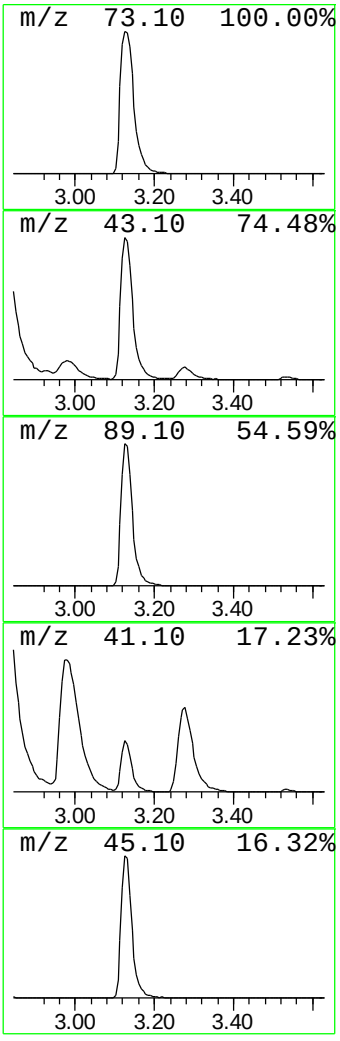
****

Peak Number 2 unknown3.13 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	378.65 ng	16244000	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	40
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	33
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





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Data File : BG024618.D
Acq On : 2 Nov 2016 8:18
Operator : UM/SJ
Sample : H5489-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-70-11.5-12.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

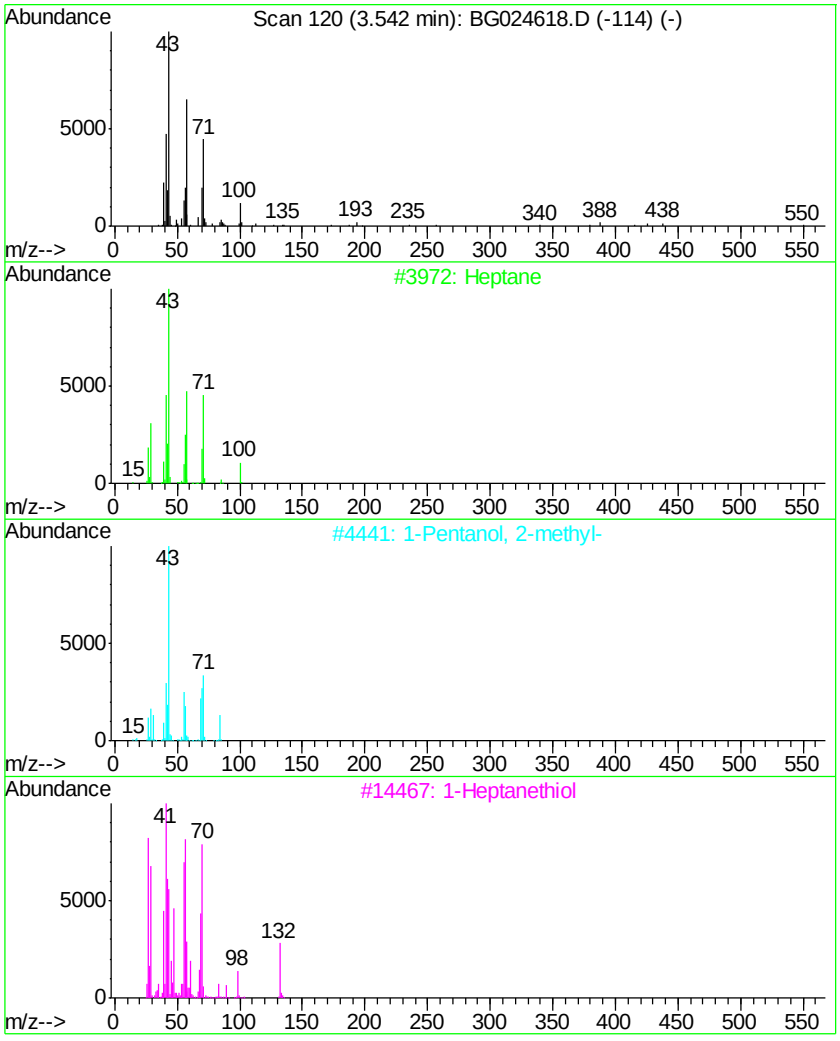
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

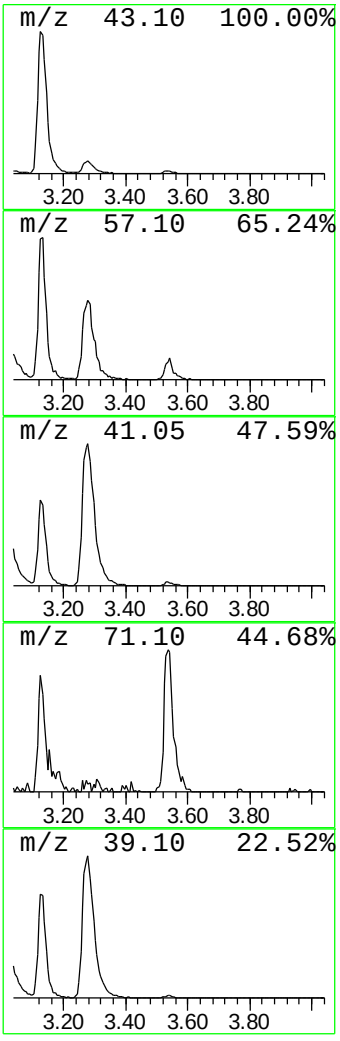
****

Peak Number 4 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	5.70 ng	244728	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	64
2	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	45
3	1-Heptanethiol	132	C7H16S	001639-09-4	23
4	Oxirane, pentyl-	114	C7H14O	005063-65-0	23
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	23





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Operator : UM/SJ
Sample : H5489-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-70-11.5-12.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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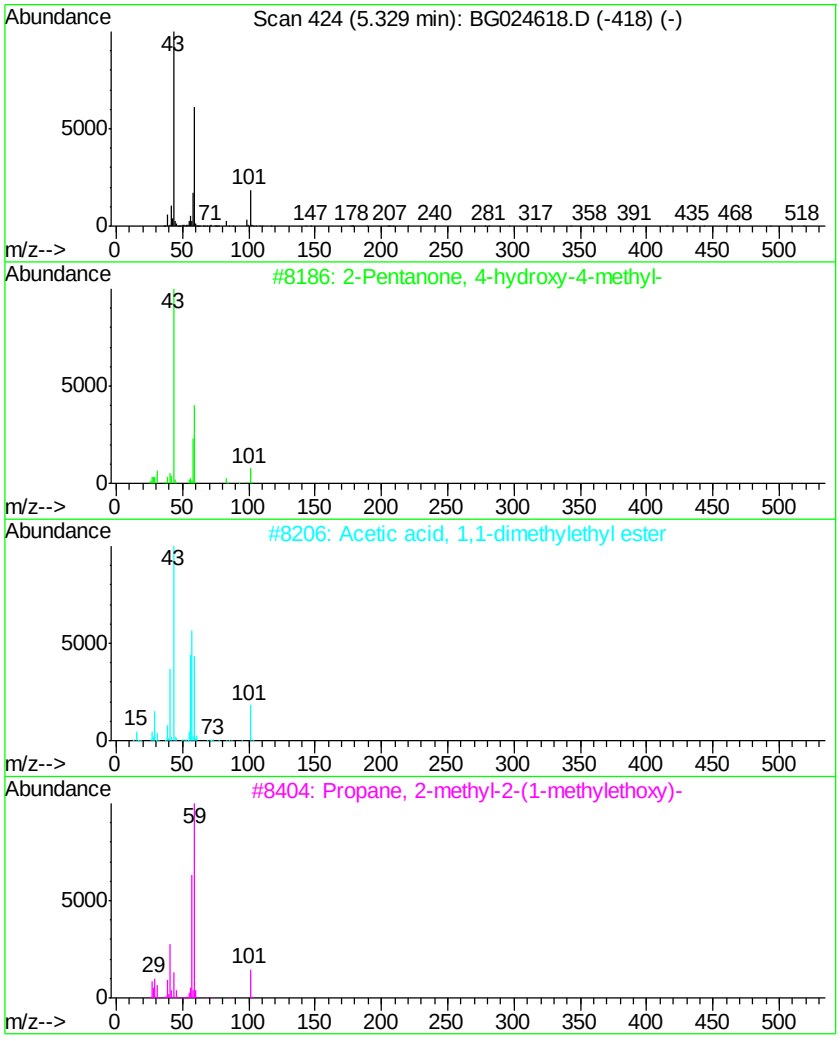
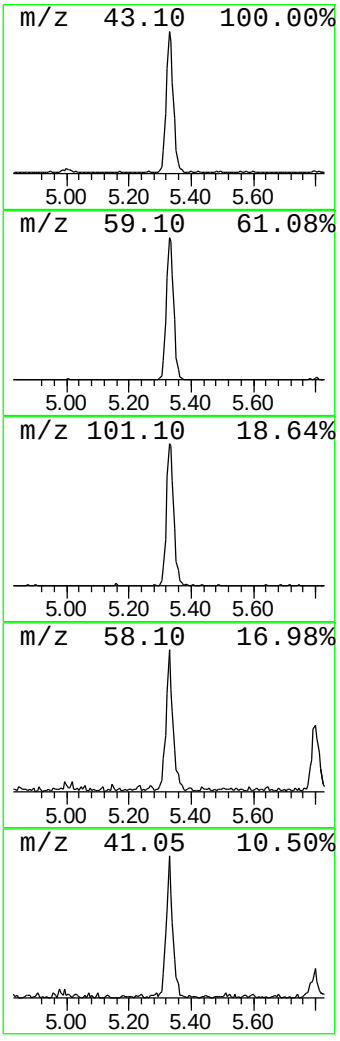
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	20.31 ng	871336	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Data File : BG024618.D
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Operator : UM/SJ
Sample : H5489-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-70-11.5-12.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

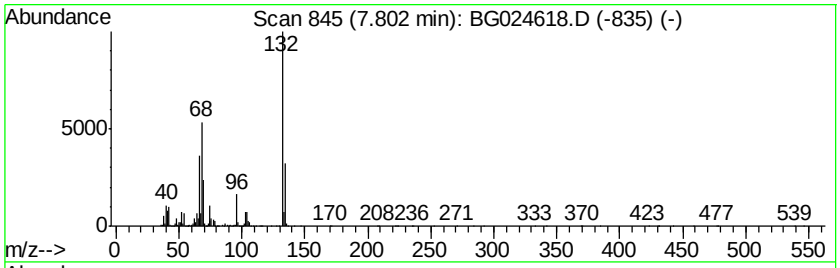
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

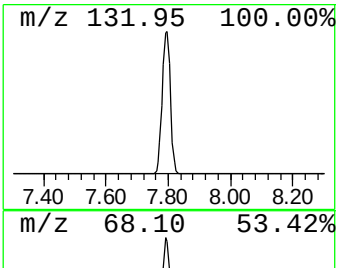
****

Peak Number 6 unknown7.80 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	98.42 ng	4222110	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





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Misc :
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Instrument : BNA_G
ClientSampleId : SB-70-11.5-12.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

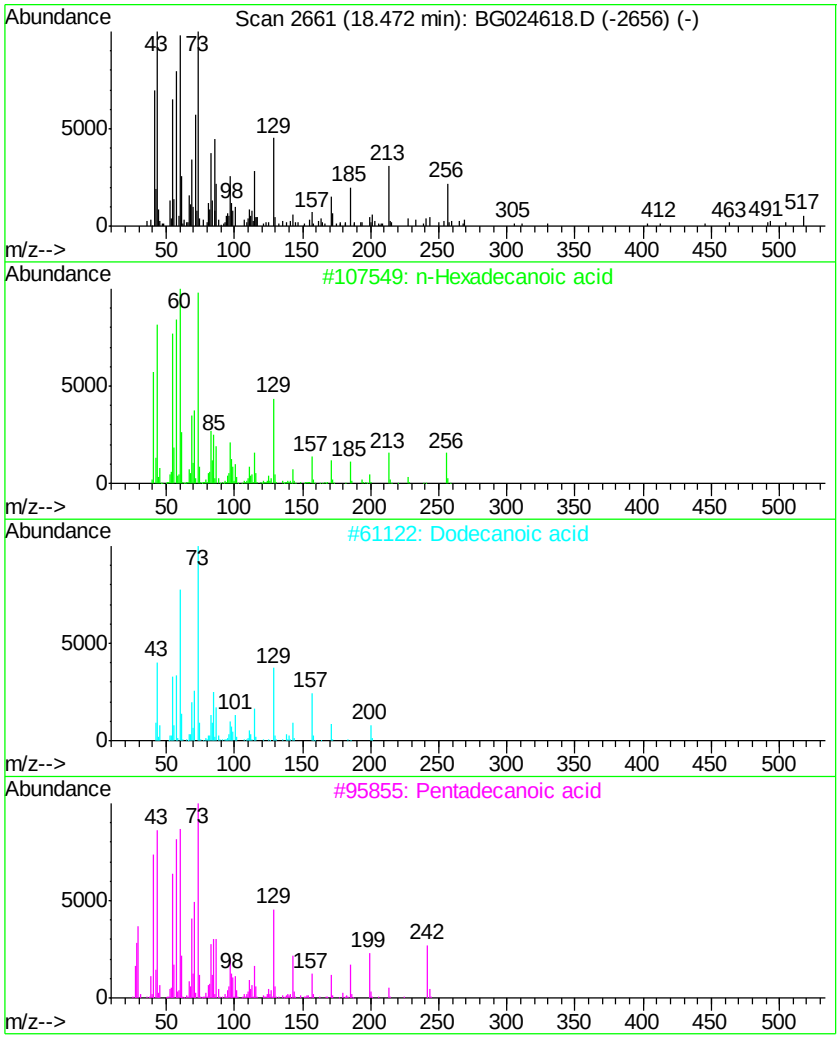
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

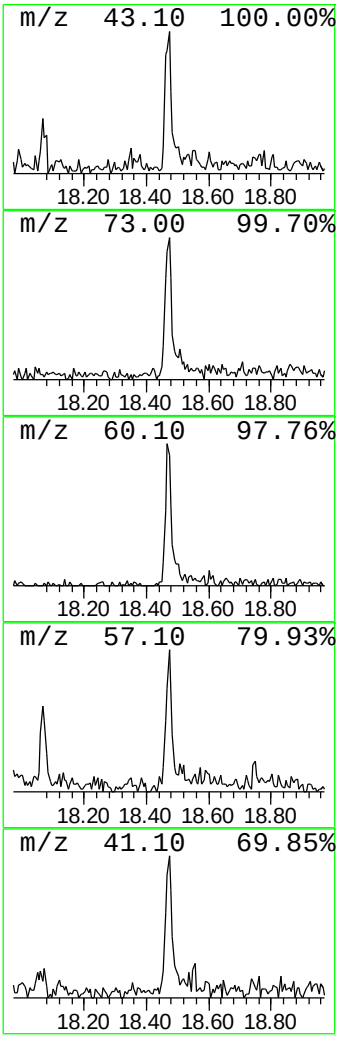
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.53 ng	254067	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Dodecanoic acid	200	C12H24O2	000143-07-7	62
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Tridecanoic acid	214	C13H26O2	000638-53-9	49





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
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ClientSampleId : SB-70-11.5-12.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

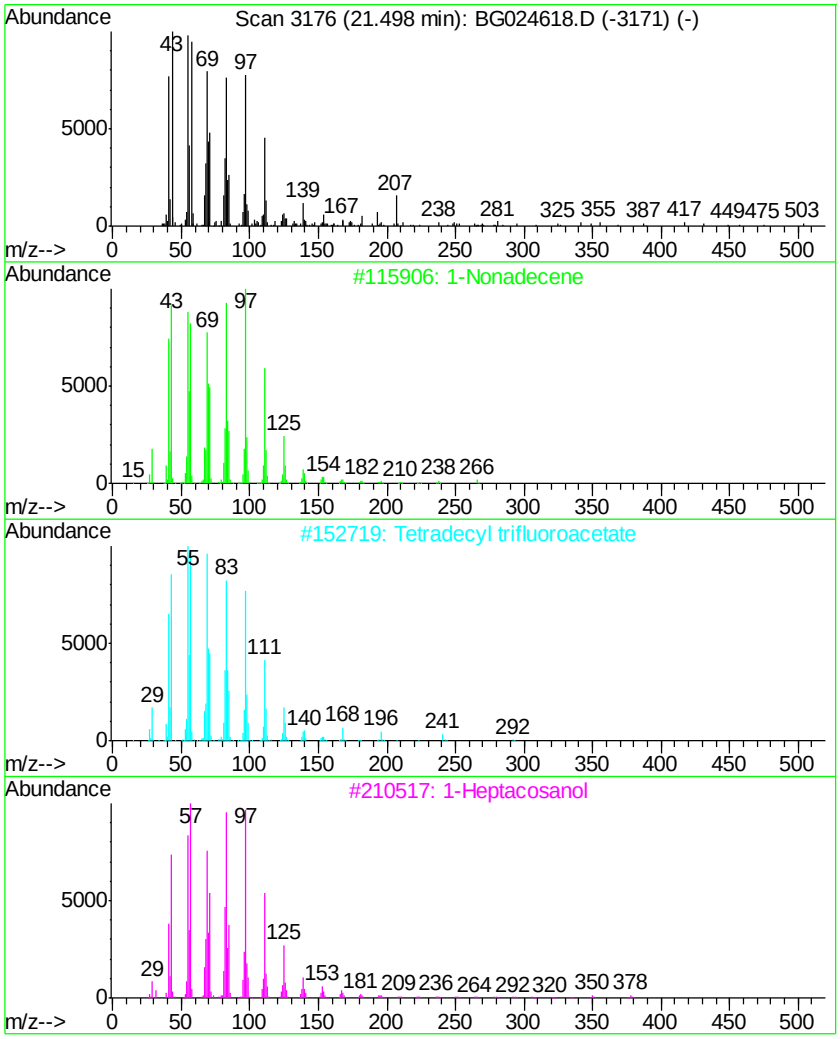
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

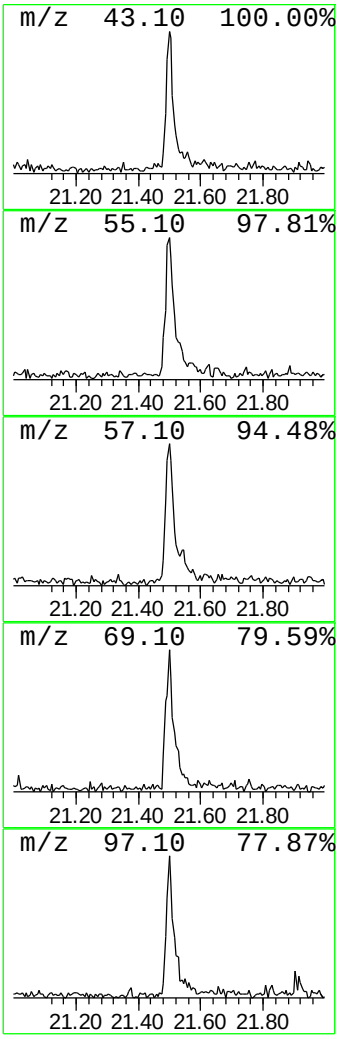
****

Peak Number 9 1-Nonadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	3.83 ng	538095	Chrysene-d12	21.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	93
2	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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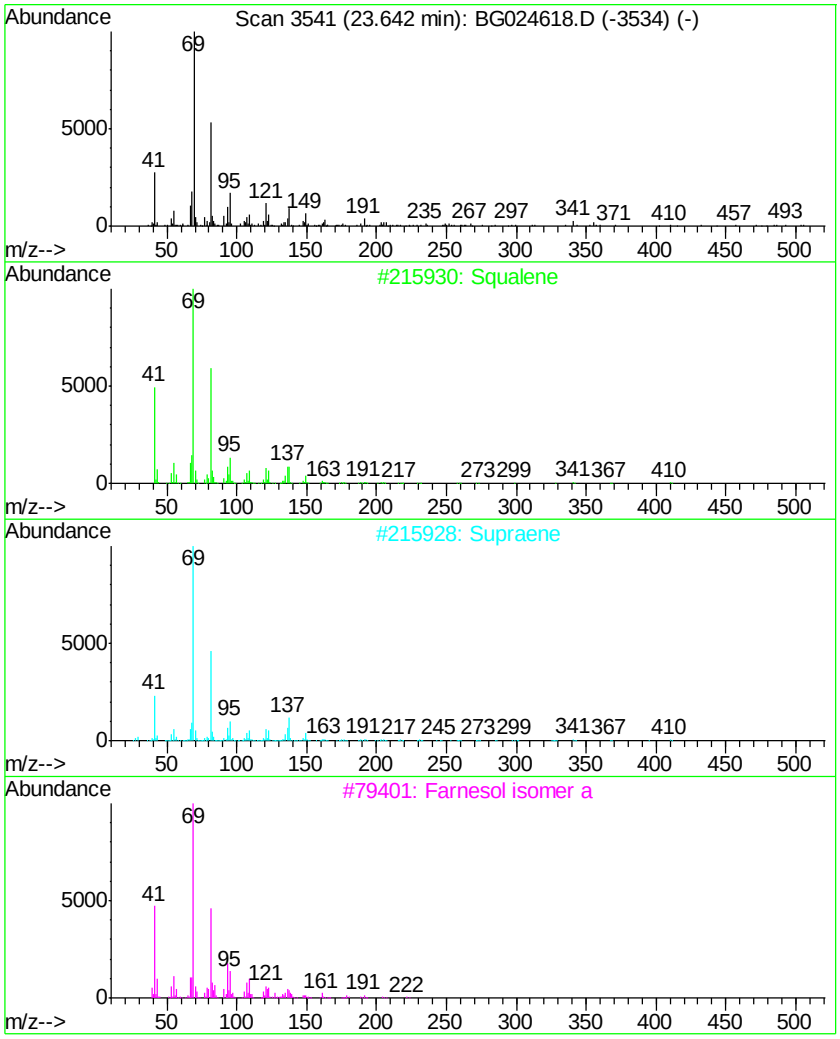
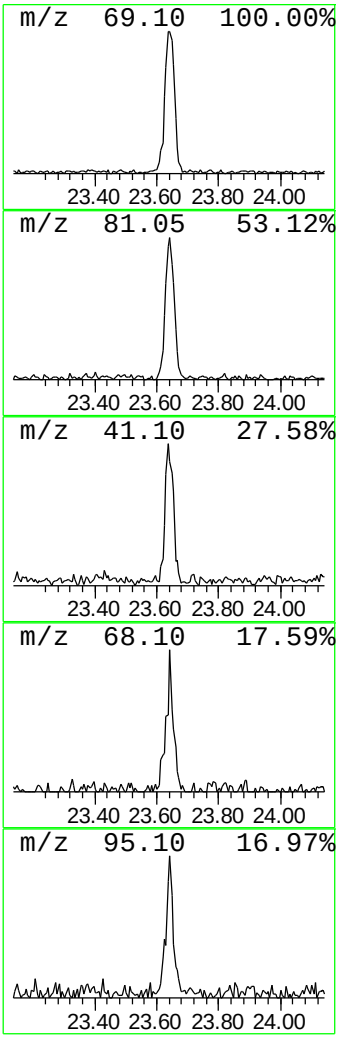
Peak Number 10 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.64	2.98 ng	428102	Perylene-d12	25.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	97
2	Supraene	410	C30H50	007683-64-9	90
3	Farnesol isomer a	222	C15H26O	1000108-92-4	56
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	56
5	Cyclopropanecarboxylic acid, 4-i...	204	C13H16O2	1000331-01-9	53





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
Cyclopentane, met...	2.98	533.8	ng	22897800	1	8.27	858003	20.0
unknown3.13	3.13	378.6	ng	16244000	1	8.27	858003	20.0
Heptane	3.54	5.7	ng	244728	1	8.27	858003	20.0
2-Pentanone, 4-hy...	5.33	20.3	ng	871336	1	8.27	858003	20.0
unknown7.80	7.80	98.4	ng	4222110	1	8.27	858003	20.0
n-Hexadecanoic acid	18.47	2.5	ng	254067	4	17.63	2008470	20.0
1-Nonadecene	21.50	3.8	ng	538095	5	21.91	2810630	20.0
Squalene	23.64	3.0	ng	428102	6	25.35	2868410	20.0