LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024605.D
Acq On : 1 Nov 2016 23:01
Operator : UM/SJ
Sample : H5489-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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	2.981	17	24	43	rVB	8942184	30599548	100.00%	22.378%
2	3.128	43	49	67	rVB	8706149	19214792	62.79%	14.052%
3	3.275	67	74	96	rVB	7202602	20996714	68.62%	15.355%
4	3.539	113	119	134	rVB3	201786	475551	1.55%	0.348%
5	5.331	418	424	432	rBV2	663515	1123027	3.67%	0.821%
6	5.801	496	504	511	rBV	2981336	5031778	16.44%	3.680%
7	7.405	767	777	788	rBV	3137974	5639799	18.43%	4.125%
8	7.793	834	843	854	rBV	2975374	5328172	17.41%	3.897%
9	8.269	916	924	936	rBV	498116	920370	3.01%	0.673%
10	8.592	972	979	990	rVB	2230893	3991841	13.05%	2.919%
11	9.444	1116	1124	1132	rBV	1909730	3497994	11.43%	2.558%
12	11.095	1397	1405	1412	rBV	638373	1177490	3.85%	0.861%
13	13.510	1803	1816	1823	rBV	4870207	7910493	25.85%	5.785%
14	14.321	1945	1954	1961	rBV	1161325	1733885	5.67%	1.268%
15	14.885	2043	2050	2057	rVB	1064388	1690144	5.52%	1.236%
16	16.365	2295	2302	2311	rBV	4524480	6970389	22.78%	5.098%
17	17.623	2509	2516	2523	rBV2	1335743	2170065	7.09%	1.587%
18	18.469	2655	2660	2668	rBV2	212134	321830	1.05%	0.235%
19	20.208	2949	2956	2962	rBV	8335281	11522423	37.66%	8.427%
20	21.500	3171	3176	3183	rBV2	242649	423300	1.38%	0.310%
21	21.918	3240	3247	3256	rVB	1635761	2830967	9.25%	2.070%
22	23.645	3534	3541	3547	rVB2	175040	360027	1.18%	0.263%
23	25.343	3819	3830	3842	rVB2	935306	2807189	9.17%	2.053%

Sum of corrected areas: 136737788

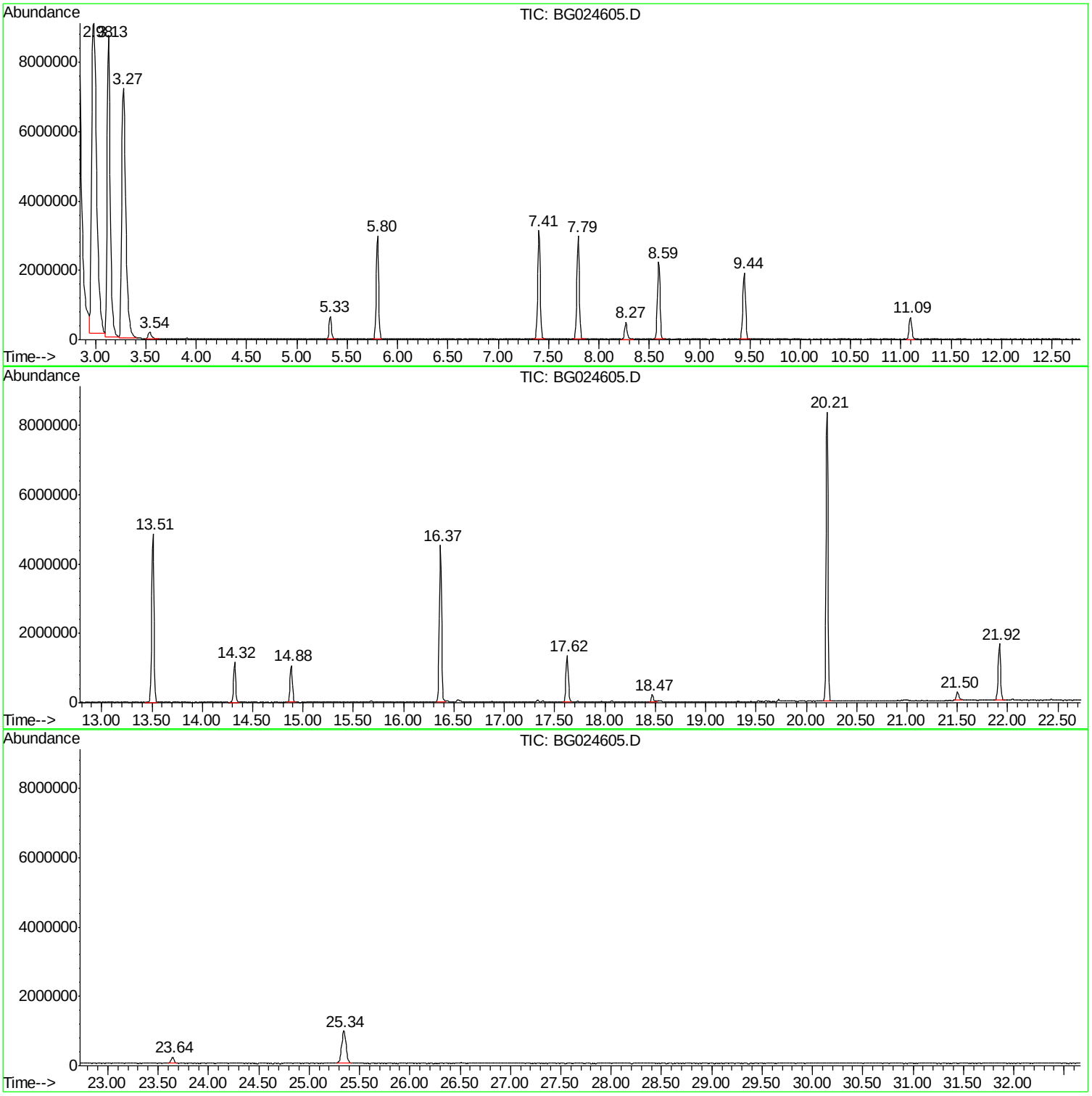
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024605.D
Acq On : 1 Nov 2016 23:01
Operator : UM/SJ
Sample : H5489-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024605.D
Acq On : 1 Nov 2016 23:01
Operator : UM/SJ
Sample : H5489-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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

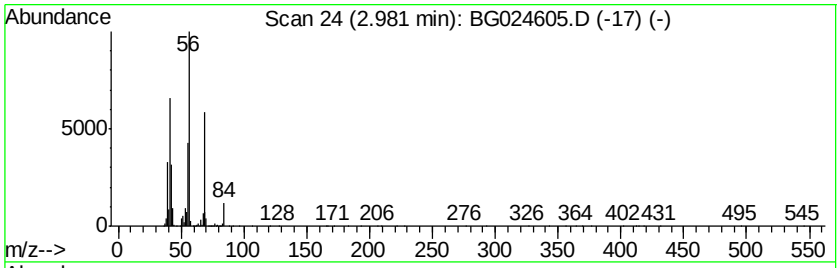
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

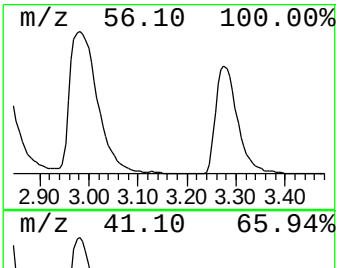
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	664.94 ng	30599500	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	80
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
4	Cyclobutane	56	C4H8	000287-23-0	50
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	45





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024605.D
Acq On : 1 Nov 2016 23:01
Operator : UM/SJ
Sample : H5489-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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

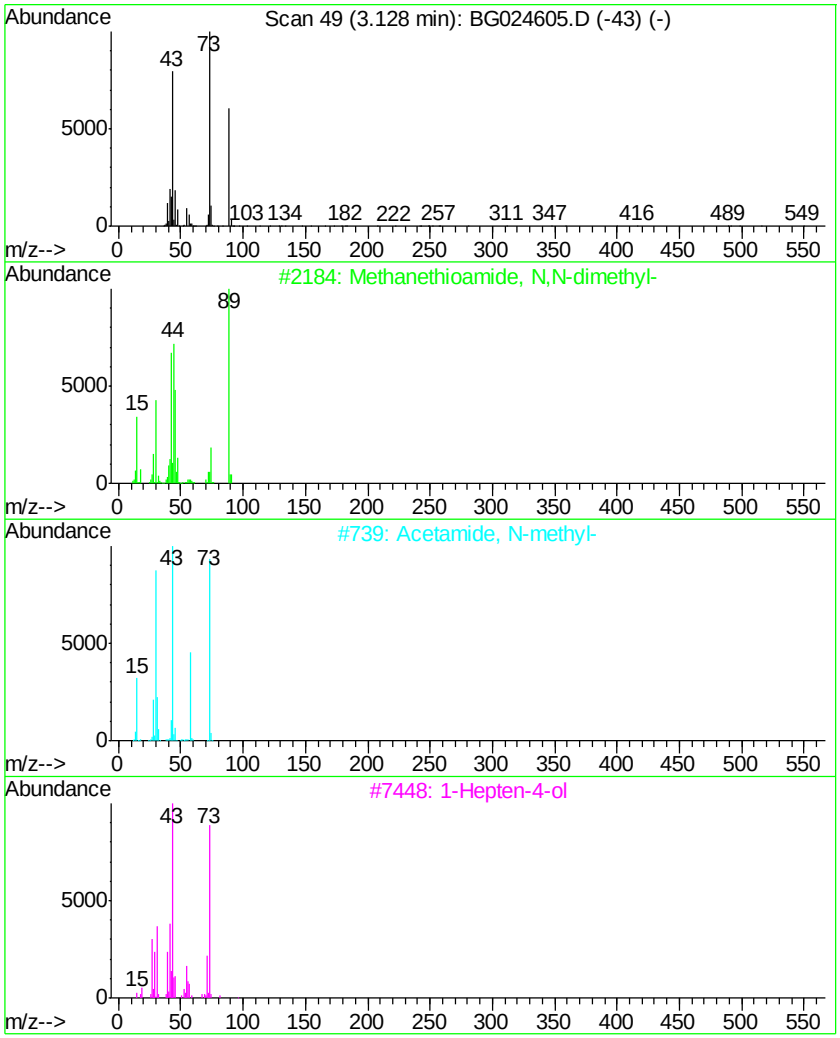
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

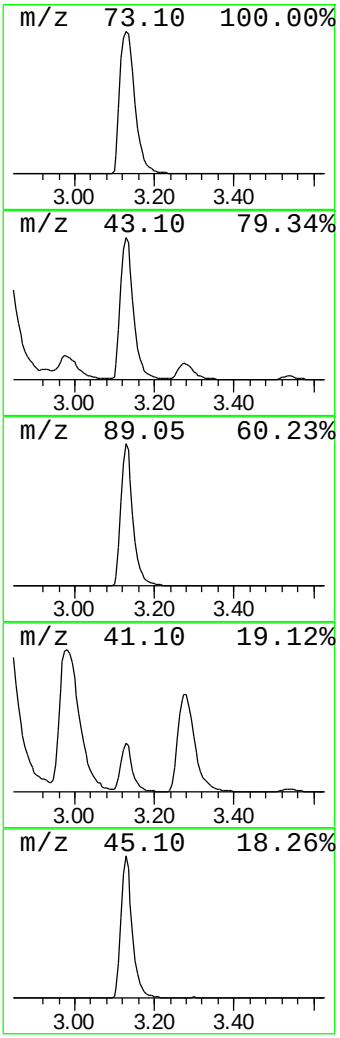
****

Peak Number 2 unknown3.13 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	417.55 ng	19214800	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	38
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3	1-Hepten-4-ol	114	C7H14O	003521-91-3	23
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5	Ethyl formate	74	C3H6O2	000109-94-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024605.D
Acq On : 1 Nov 2016 23:01
Operator : UM/SJ
Sample : H5489-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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

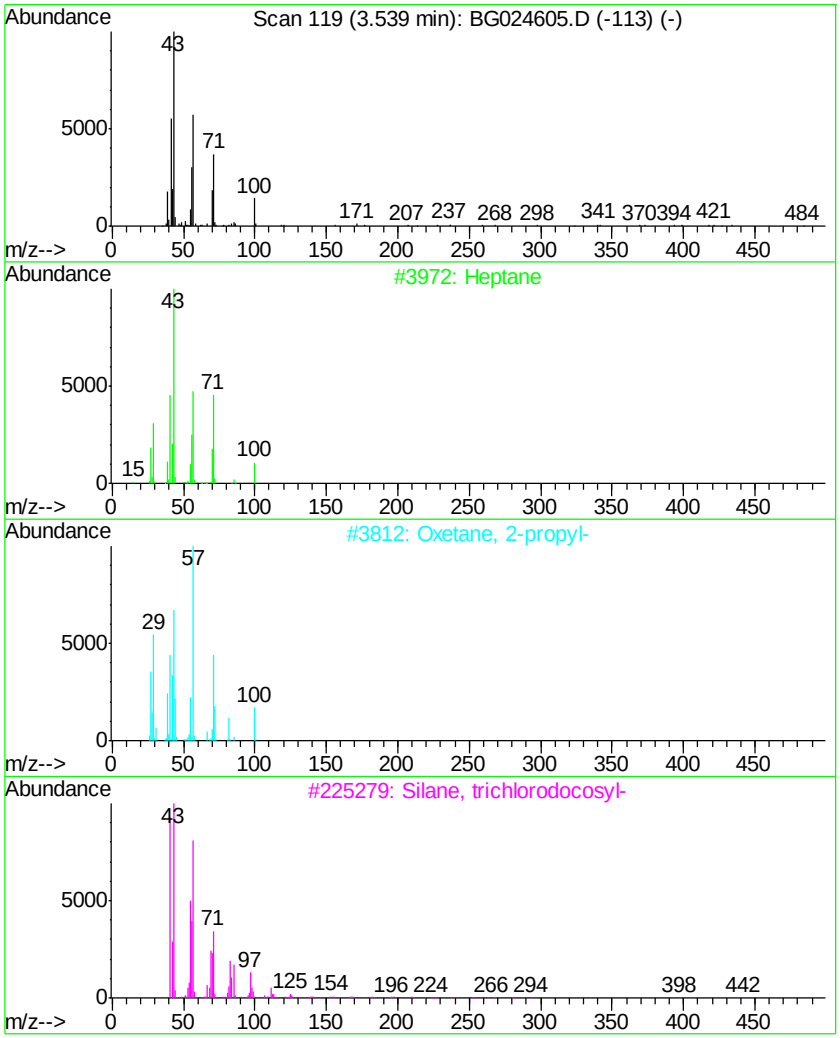
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

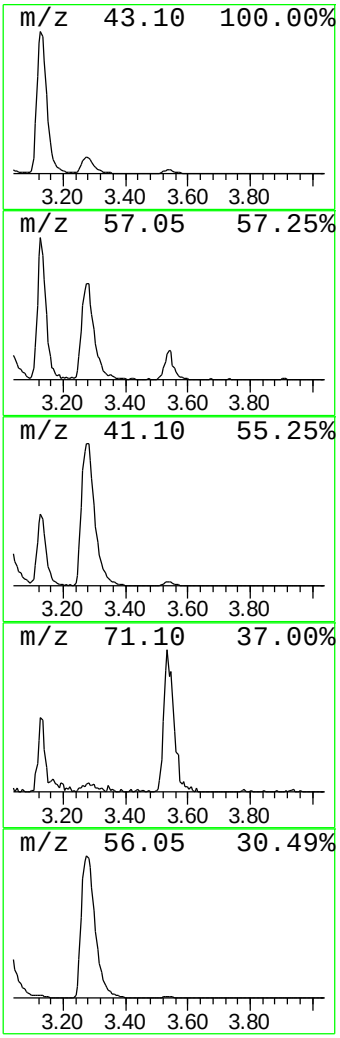
****

Peak Number 4 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	10.33 ng	475551	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	87
2	Oxetane, 2-propyl-	100	C6H12O	004468-64-8	47
3	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	38
4	Decane, 2-methyl-	156	C11H24	006975-98-0	28
5	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	25





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024605.D
Acq On : 1 Nov 2016 23:01
Operator : UM/SJ
Sample : H5489-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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

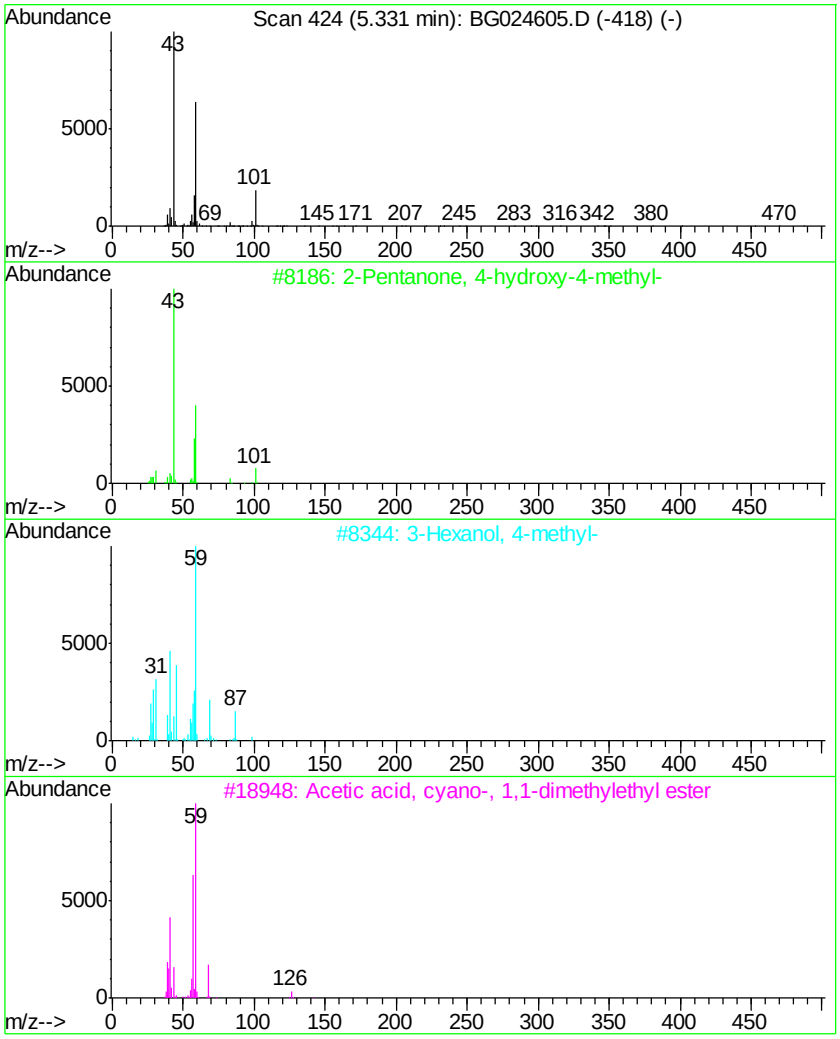
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

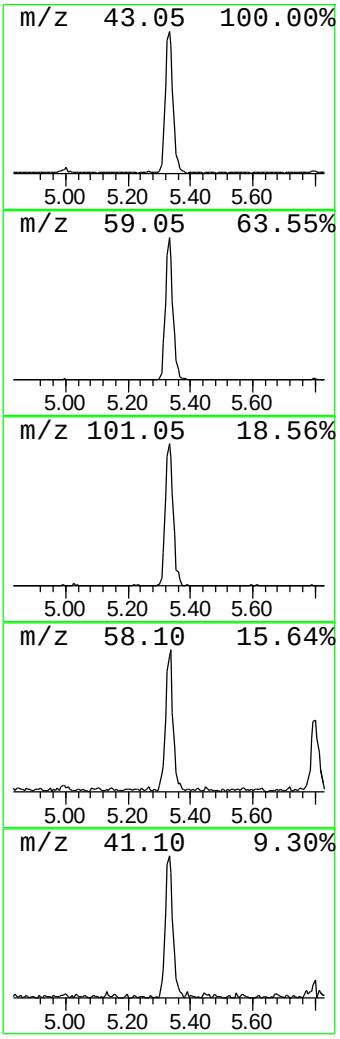
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	24.40 ng	1123030	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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024605.D
Acq On : 1 Nov 2016 23:01
Operator : UM/SJ
Sample : H5489-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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

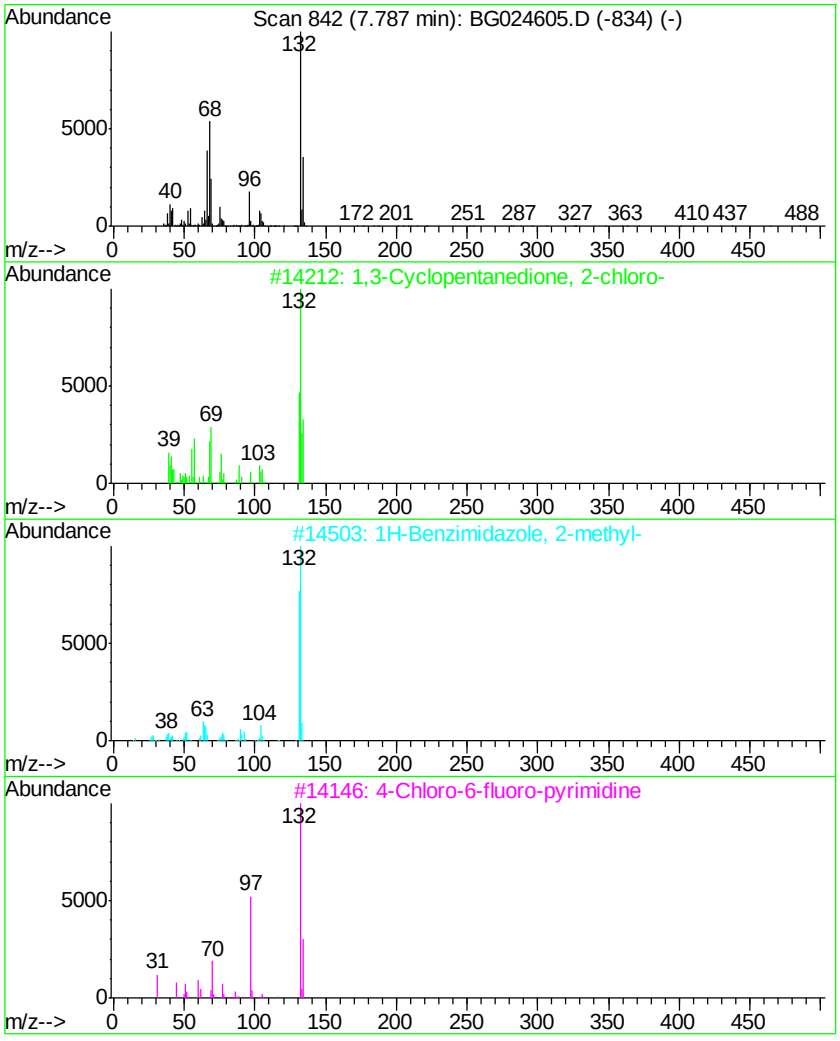
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

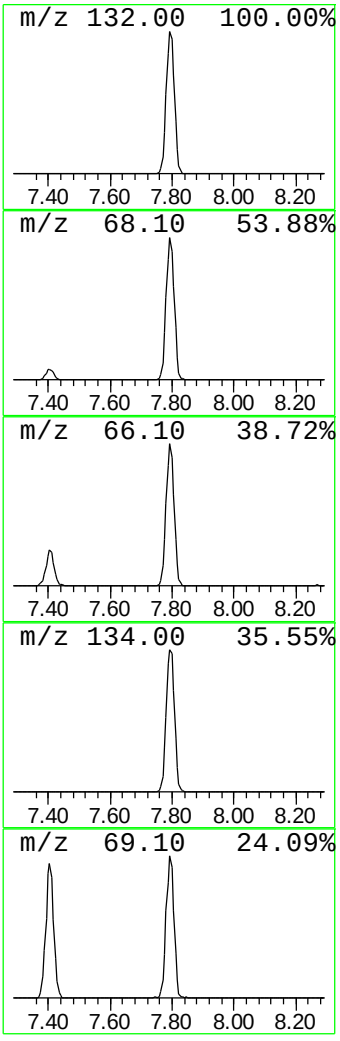
****

Peak Number 6 unknown7.79 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	115.78 ng	5328170	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
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Operator : UM/SJ
Sample : H5489-09
Misc :
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Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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

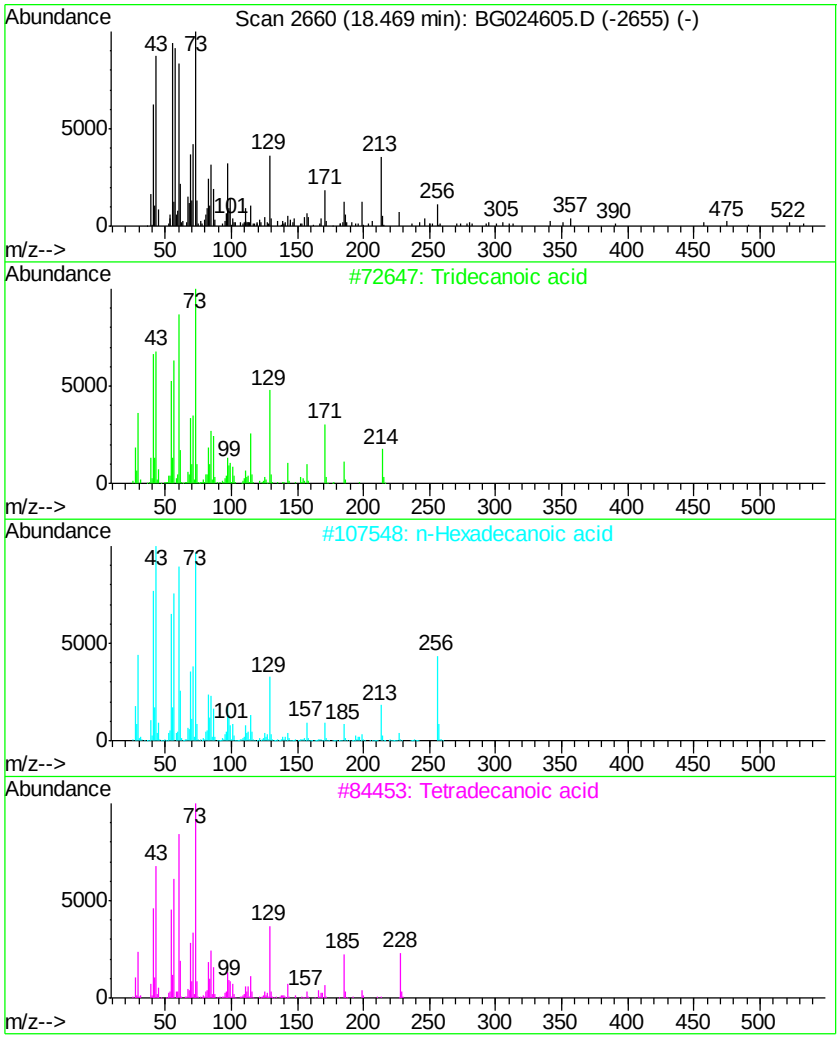
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

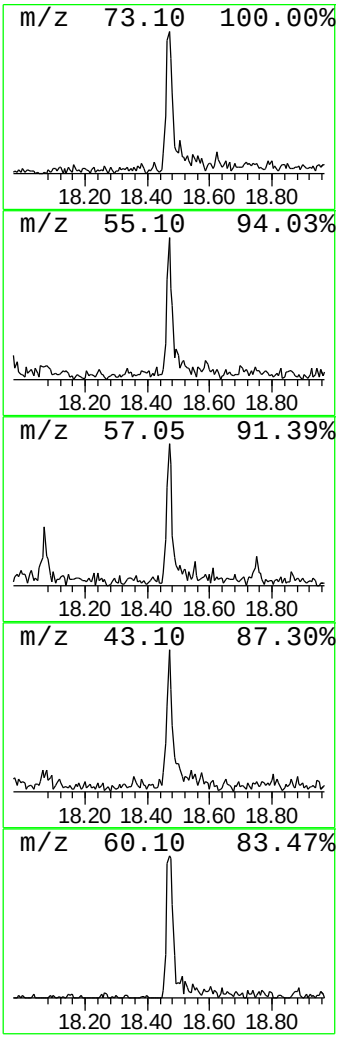
****

Peak Number 8 Tridecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.97 ng	321830	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





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Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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

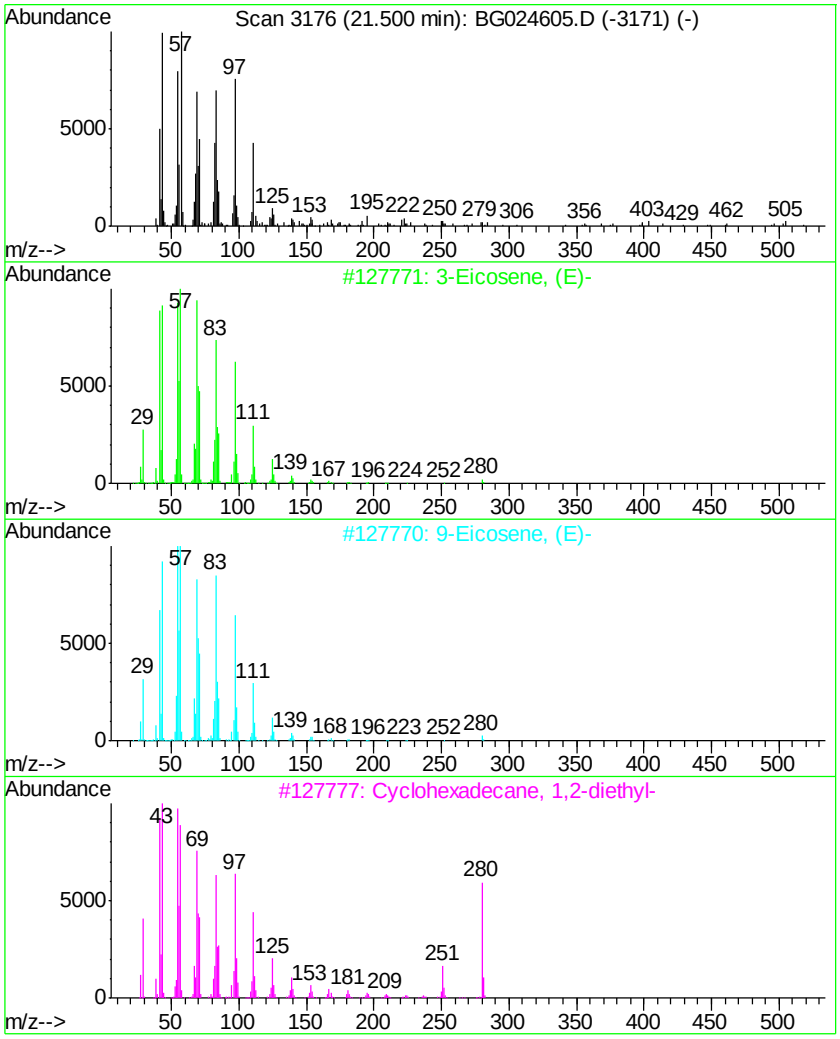
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

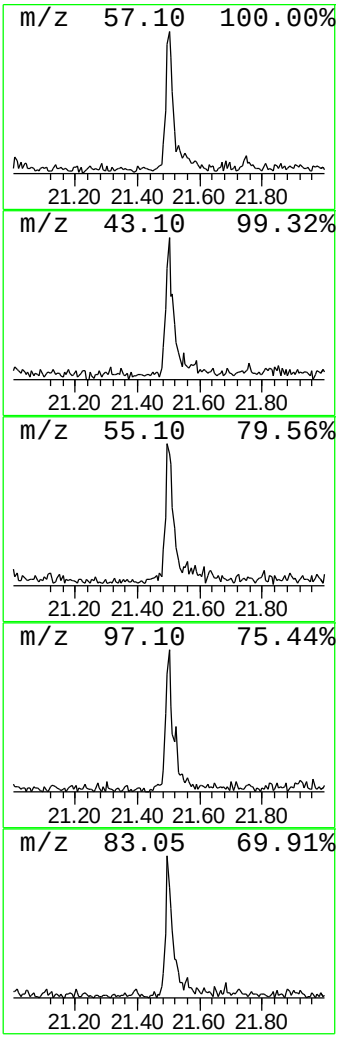
****

Peak Number 9 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	2.99 ng	423300	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	86
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	53
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	50
4	Cyclopentadecane	210	C15H30	000295-48-7	49
5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	49





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
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Operator : UM/SJ
Sample : H5489-09
Misc :
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Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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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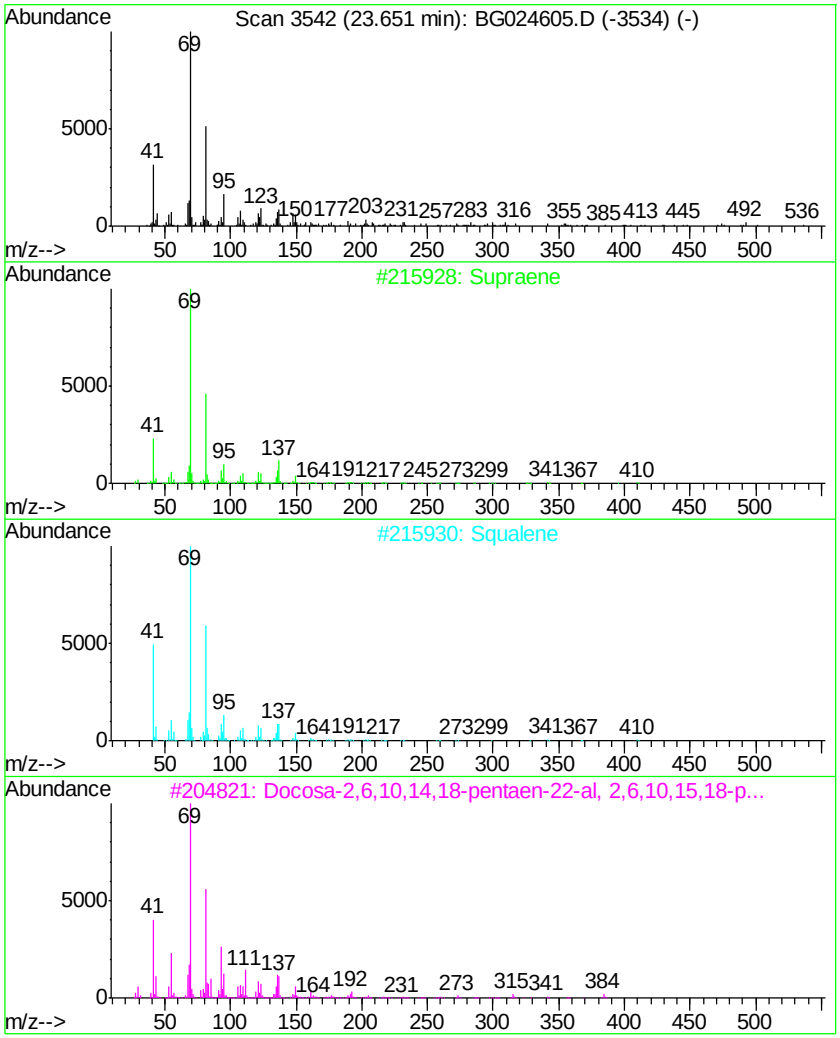
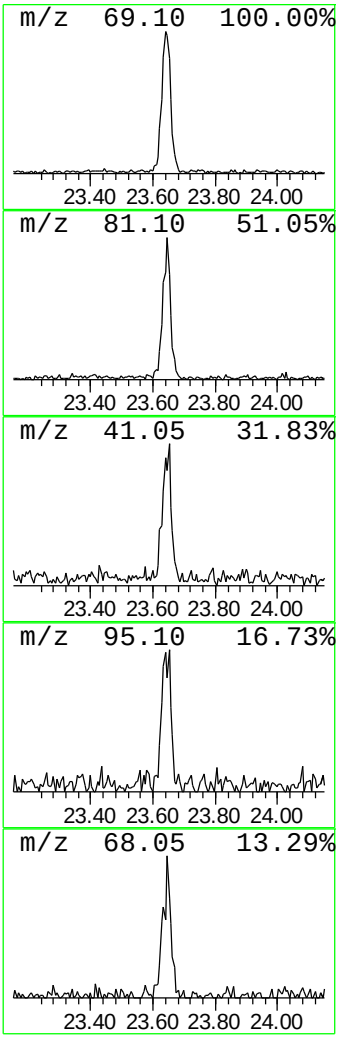
Peak Number 10 Supraene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.65	2.57 ng	360027	Perylene-d12	25.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	93
2	Squalene	410	C30H50	000111-02-4	93
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4	2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	003675-00-1	72
5	Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110116\
Data File : BG024605.D
Acq On : 1 Nov 2016 23:01
Operator : UM/SJ
Sample : H5489-09
Misc :
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Instrument : BNA_G
ClientSampleId : SB-71-13.5-14

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, met...	2.98	664.9	ng	30599500	1	8.27	920370	20.0
unknown3.13	3.13	417.6	ng	19214800	1	8.27	920370	20.0
Heptane	3.54	10.3	ng	475551	1	8.27	920370	20.0
2-Pentanone, 4-hy...	5.33	24.4	ng	1123030	1	8.27	920370	20.0
unknown7.79	7.79	115.8	ng	5328170	1	8.27	920370	20.0
Tridecanoic acid	18.47	3.0	ng	321830	4	17.62	2170070	20.0
3-Eicosene, (E)-	21.50	3.0	ng	423300	5	21.92	2830970	20.0
Supraene	23.65	2.6	ng	360027	6	25.34	2807190	20.0