LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024619.D
Acq On : 2 Nov 2016 8:56
Operator : UM/SJ
Sample : H5489-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-72-0.5-1.0

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	2.979	18	24	44	rVB	8443308	26413311	100.00%	21.069%
2	3.126	44	49	67	rVB	8000657	15593884	59.04%	12.439%
3	3.273	67	74	100	rVB	7229204	18832653	71.30%	15.022%
4	3.532	114	118	130	rVB3	216982	437810	1.66%	0.349%
5	5.330	417	424	434	rBV2	671213	1095953	4.15%	0.874%
6	5.800	496	504	513	rBV	2771943	4720028	17.87%	3.765%
7	7.404	769	777	791	rBV	3022089	5343006	20.23%	4.262%
8	7.791	834	843	853	rBV	2800119	5055114	19.14%	4.032%
9	8.267	916	924	935	rBV	465228	842460	3.19%	0.672%
10	8.591	971	979	989	rVB	2139642	3882429	14.70%	3.097%
11	9.442	1115	1124	1132	rBV	1820947	3409257	12.91%	2.719%
12	11.093	1398	1405	1414	rBV	610051	1119423	4.24%	0.893%
13	13.508	1807	1816	1825	rBV	4732233	7408283	28.05%	5.909%
14	14.319	1948	1954	1961	rBV	1204363	1796159	6.80%	1.433%
15	14.883	2043	2050	2058	rBV2	991406	1561961	5.91%	1.246%
16	16.364	2294	2302	2316	rBV	4054776	6524021	24.70%	5.204%
17	17.627	2510	2517	2528	rVB2	1216040	1977069	7.49%	1.577%
18	18.467	2655	2660	2669	rBV	204199	340145	1.29%	0.271%
19	20.206	2949	2956	2962	rBV	9097689	12461128	47.18%	9.940%
20	21.499	3171	3176	3187	rBV2	190689	360171	1.36%	0.287%
21	21.916	3240	3247	3255	rBV	1632227	2806355	10.62%	2.239%
22	23.643	3533	3541	3547	rBV2	239917	475889	1.80%	0.380%
23	25.347	3818	3831	3846	rVB3	907417	2909793	11.02%	2.321%

Sum of corrected areas: 125366302

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
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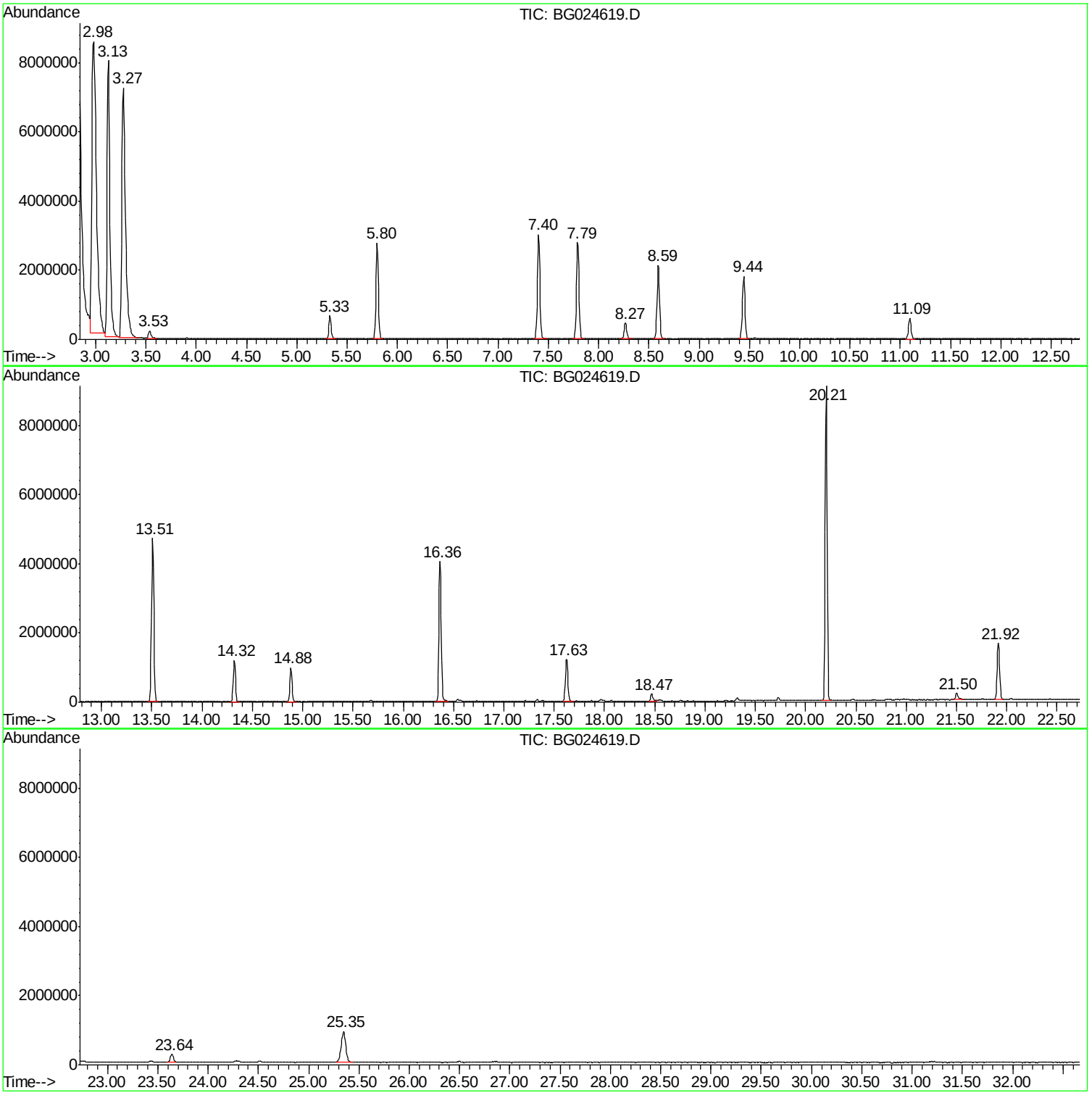
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-72-0.5-1.0

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



Library Search Compound Report

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Data File : BG024619.D
Acq On : 2 Nov 2016 8:56
Operator : UM/SJ
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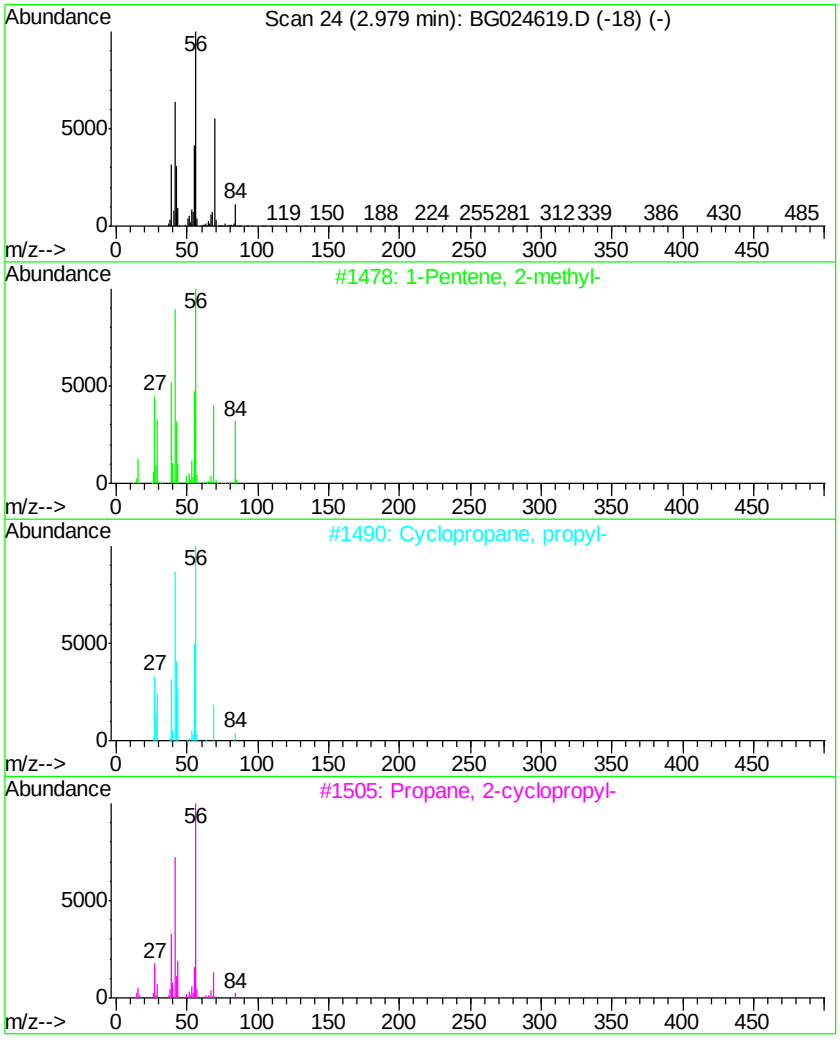
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

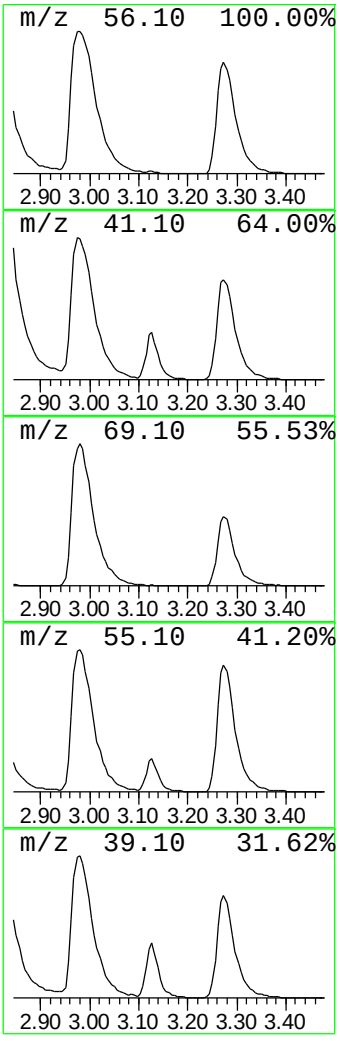
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	627.05 ng	26413300	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	56
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	53
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
5	Cyclobutane	56	C4H8	000287-23-0	50





Library Search Compound Report

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Data File : BG024619.D
Acq On : 2 Nov 2016 8:56
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Misc :
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Instrument : BNA_G
ClientSampleId : SB-72-0.5-1.0

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

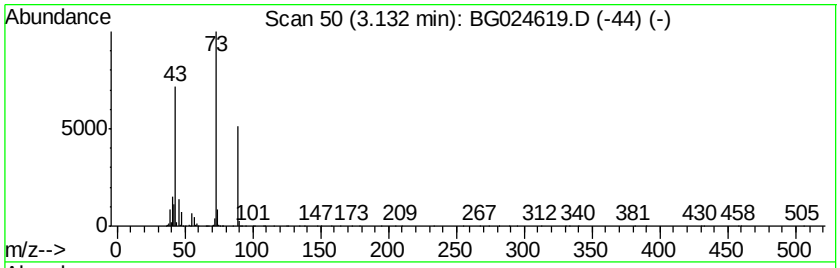
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

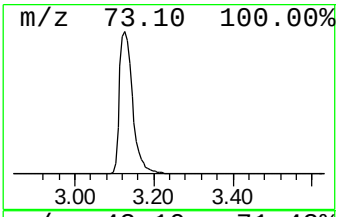
****

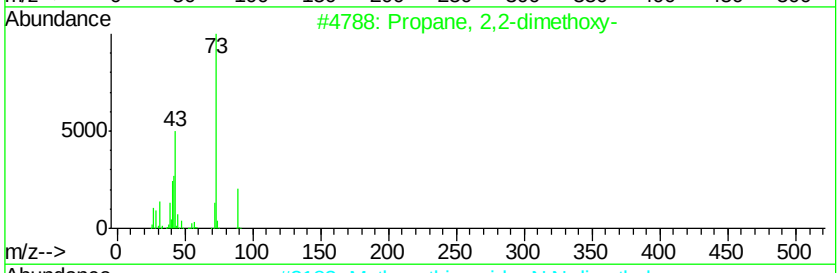
Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 3

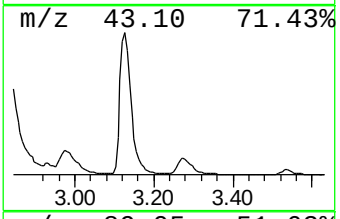
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	370.20 ng	15593900	1,4-Dichlorobenzene-d4	8.27

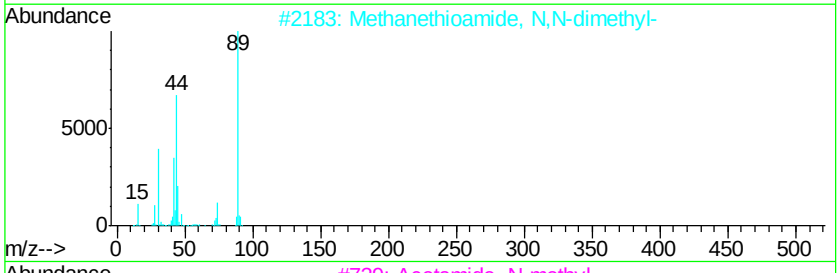
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	37
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4	1-Hepten-4-ol	114	C7H14O	003521-91-3	23
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10

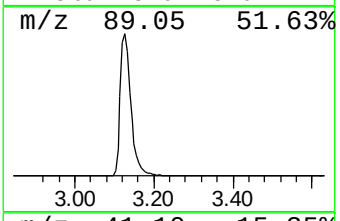


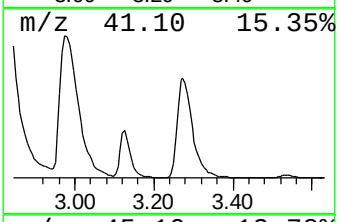


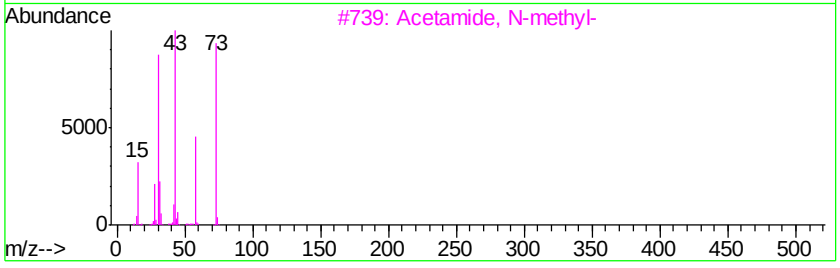


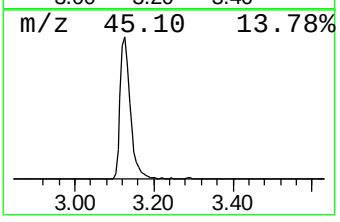












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Data File : BG024619.D
Acq On : 2 Nov 2016 8:56
Operator : UM/SJ
Sample : H5489-10
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-72-0.5-1.0

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

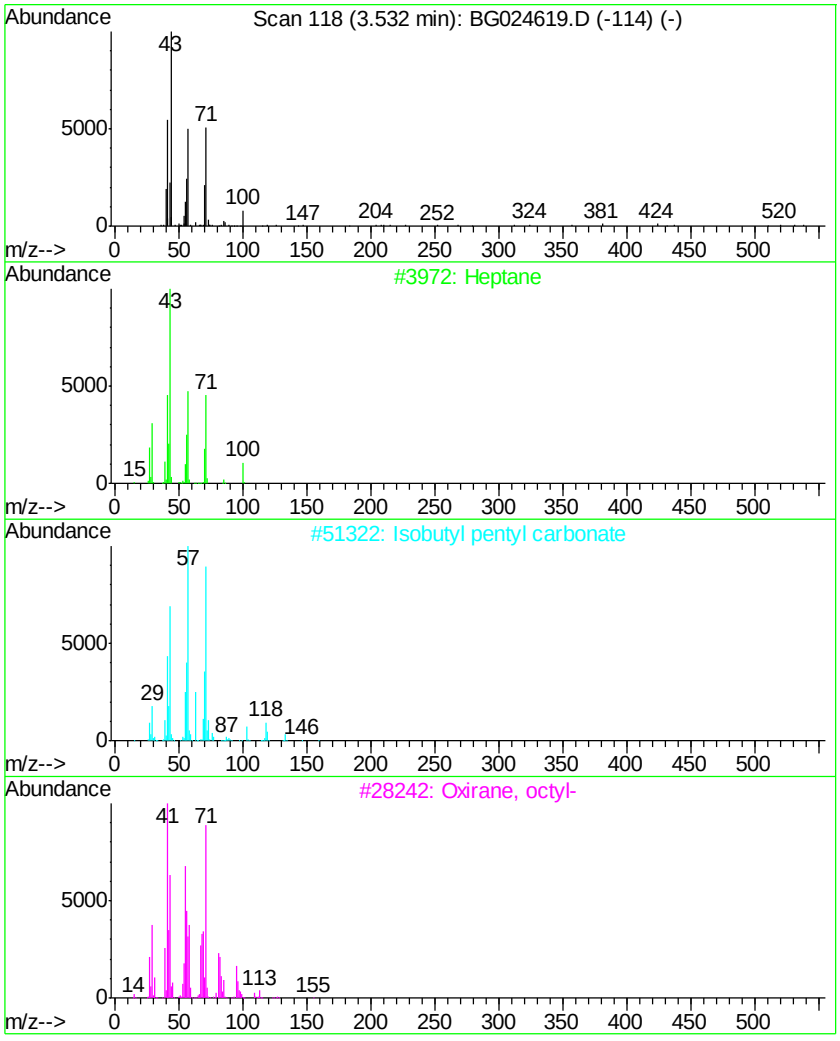
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

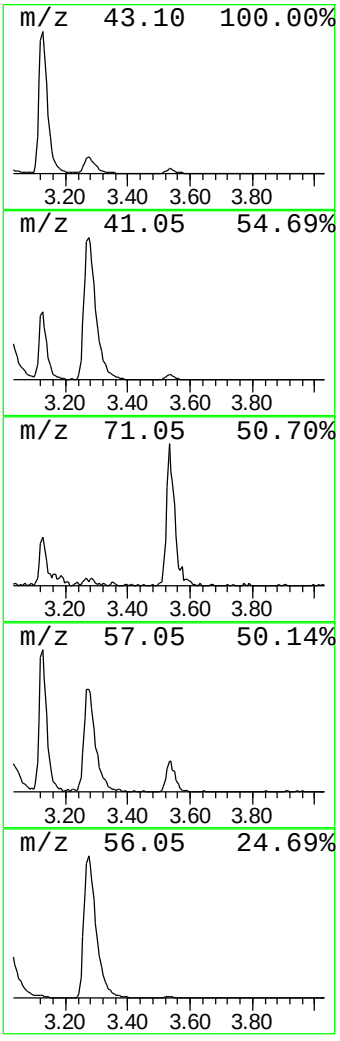
****

Peak Number 4 Heptane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	10.39 ng	437810	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	87
2	Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	42
3	Oxirane, octyl-	156	C10H20O	002404-44-6	42
4	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	38
5	Decane, 4-methyl-	156	C11H24	002847-72-5	38





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
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TIC Library : C:\DATABASE\NIST11.L
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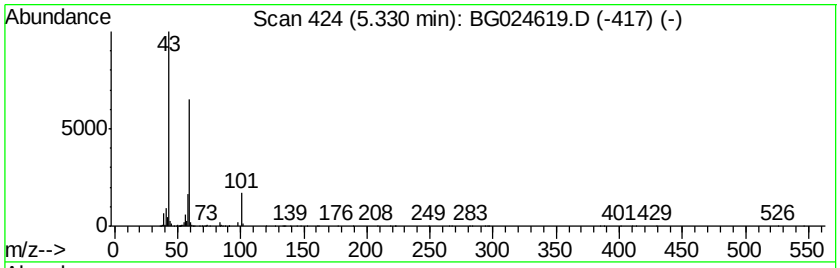
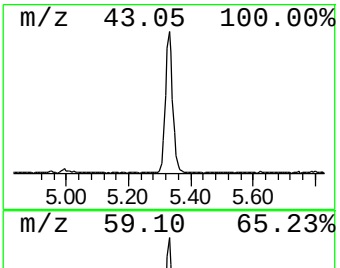
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	26.02 ng	1095950	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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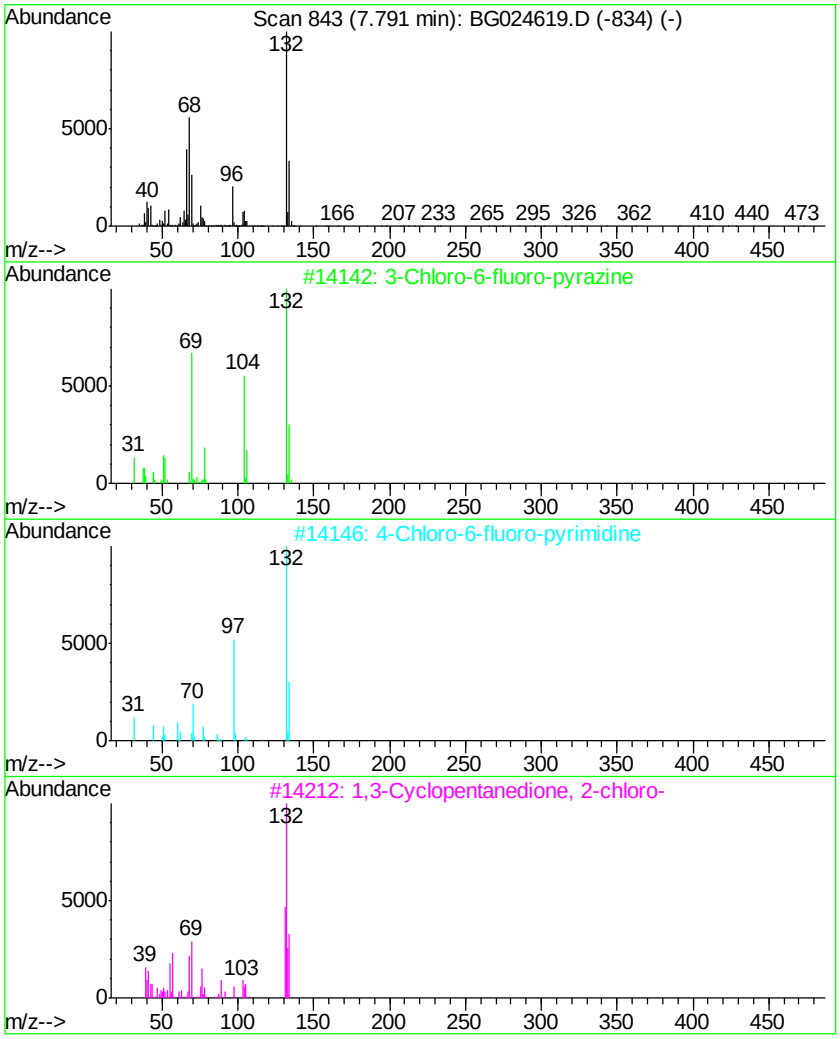
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

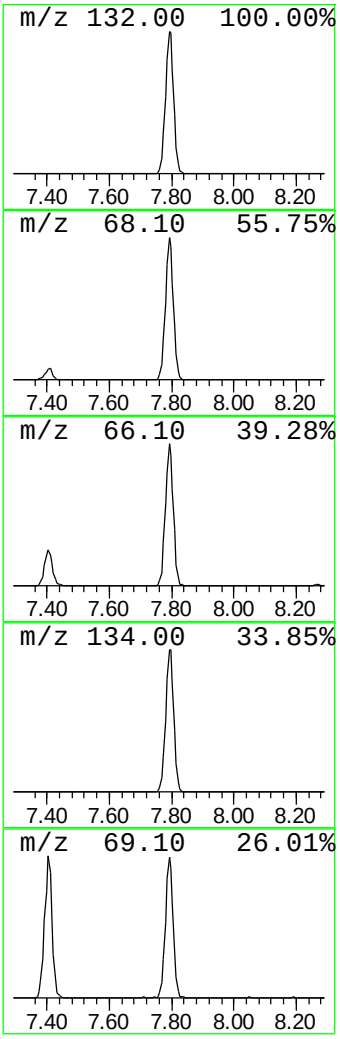
****

Peak Number 6 unknown7.79 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	120.01 ng	5055110	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10





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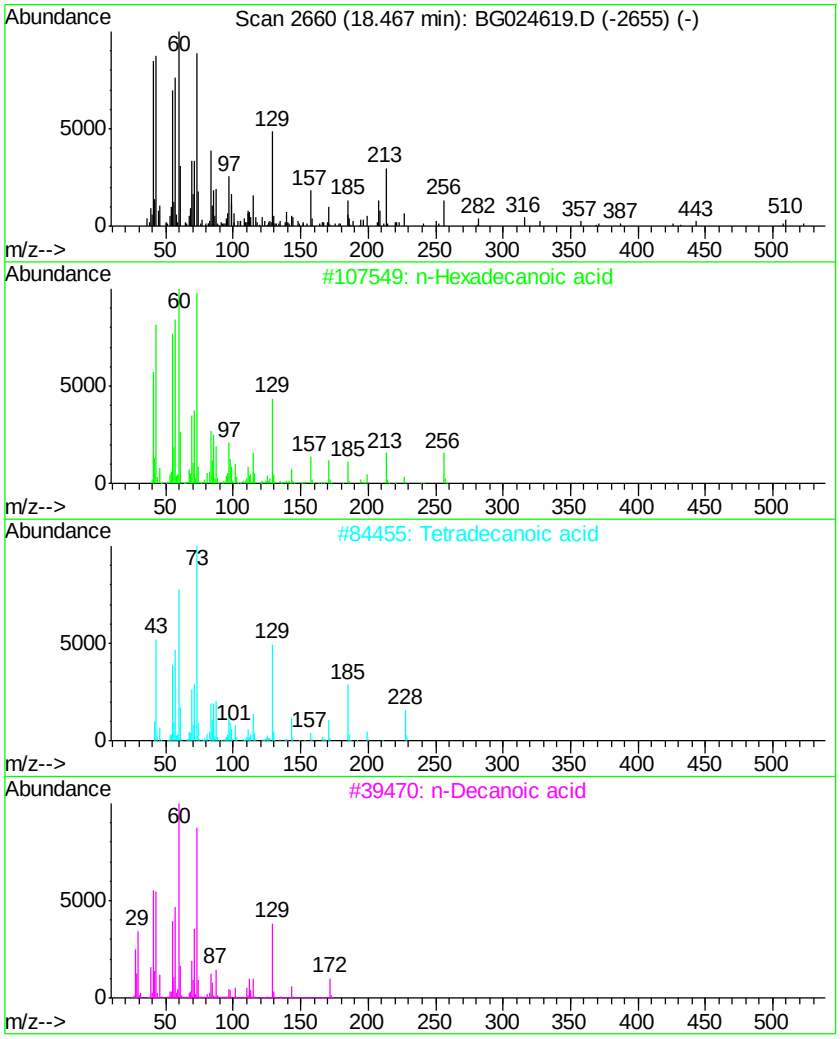
TIC Integration Parameters: LSCINT.P

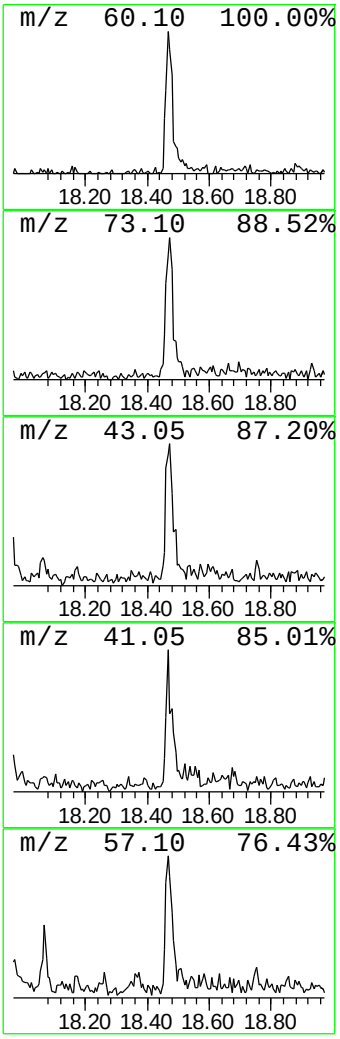
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	3.44 ng	340145	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	43





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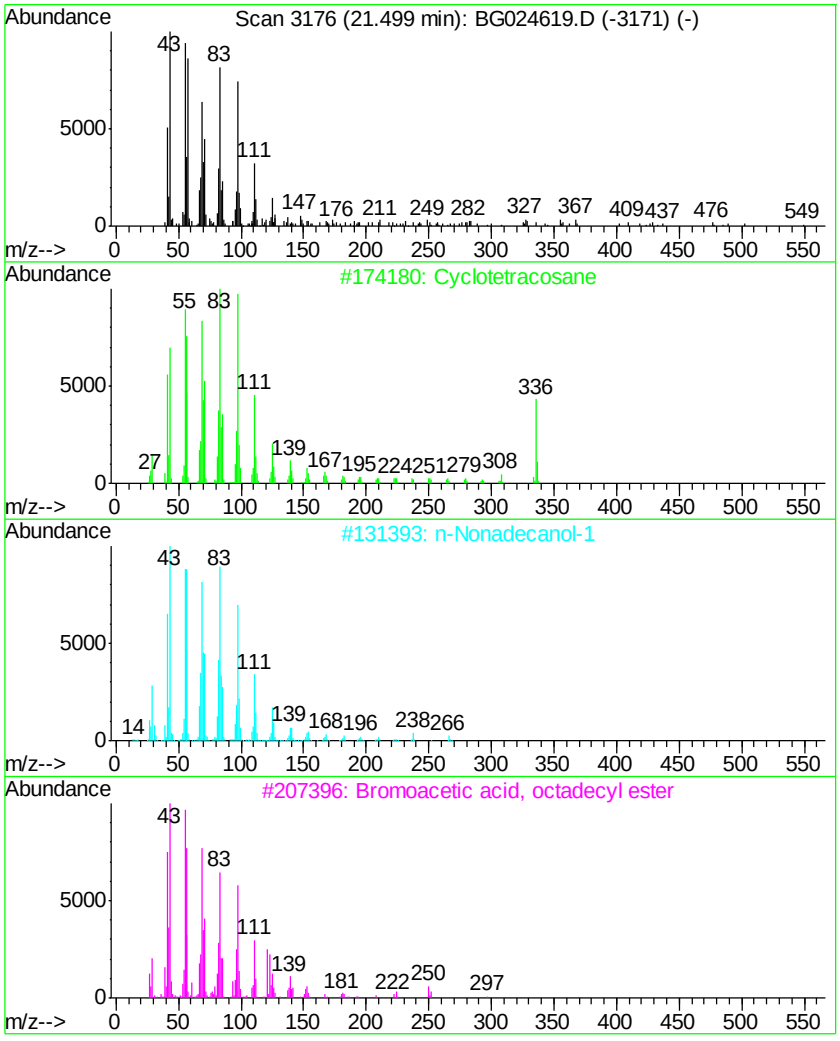
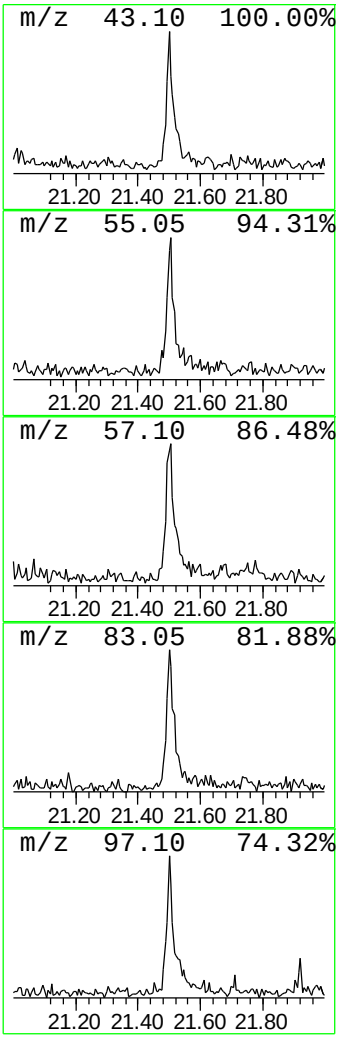
****

Peak Number 9 Cyclotetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	2.57 ng	360171	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	96
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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ClientSampleId : SB-72-0.5-1.0

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

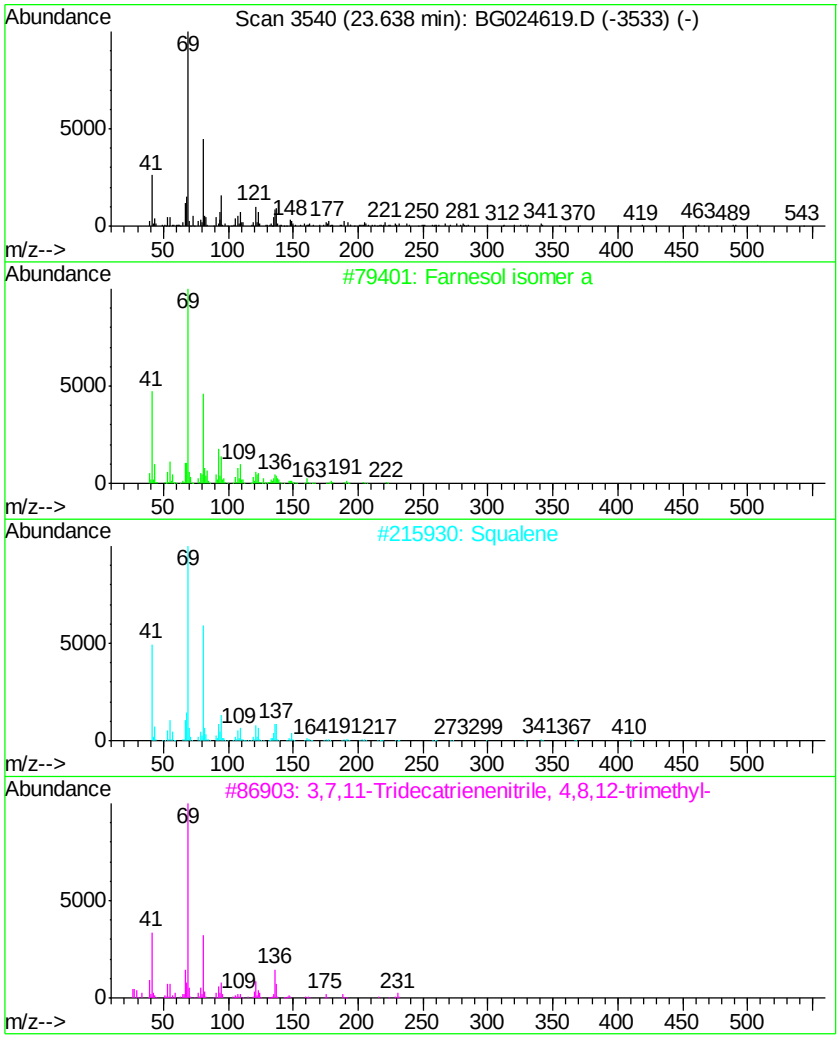
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

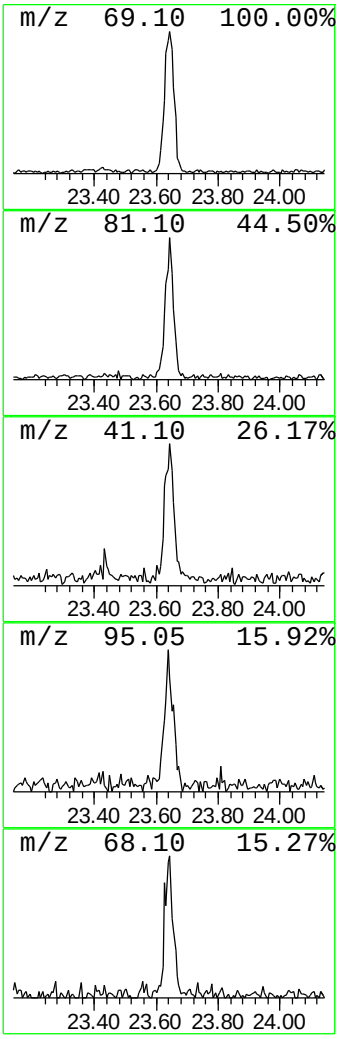
****

Peak Number 10 Farnesol isomer a Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.64	3.27 ng	475889	Perylene-d12	25.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	93
2	Squalene	410	C30H50	000111-02-4	83
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	80
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	56





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Pentene, 2-methyl-	2.98	627.0	ng	26413300	1	8.27	842460	20.0
Propane, 2,2-dime...	3.13	370.2	ng	15593900	1	8.27	842460	20.0
Heptane	3.53	10.4	ng	437810	1	8.27	842460	20.0
2-Pentanone, 4-hy...	5.33	26.0	ng	1095950	1	8.27	842460	20.0
unknown7.79	7.79	120.0	ng	5055110	1	8.27	842460	20.0
n-Hexadecanoic acid	18.47	3.4	ng	340145	4	17.63	1977070	20.0
Cyclotetracosane	21.50	2.6	ng	360171	5	21.92	2806360	20.0
Farnesol isomer a	23.64	3.3	ng	475889	6	25.35	2909790	20.0