LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023135.D
Acq On : 16 Jul 2016 6:57
Operator : UM/SJ
Sample : H4015-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-22

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	2.894	4	9	27	rVB	676101	1566564	19.09%	2.764%
2	3.041	29	34	53	rVV	3393601	5066080	61.73%	8.938%
3	3.188	53	59	74	rVV	615484	1224934	14.93%	2.161%
4	5.220	397	405	414	rBV	252546	403134	4.91%	0.711%
5	5.696	479	486	496	rBV	1947462	3141378	38.28%	5.542%
6	7.306	753	760	770	rBV	2226311	3954533	48.19%	6.977%
7	7.682	815	824	828	rBV	2039018	3590047	43.75%	6.334%
8	7.723	828	831	841	rVB	422266	645209	7.86%	1.138%
9	8.146	895	903	912	rBV	370721	647394	7.89%	1.142%
10	8.476	949	959	968	rBV	1408630	2459307	29.97%	4.339%
11	9.322	1094	1103	1113	rBV	1392274	2542186	30.98%	4.485%
12	10.978	1377	1385	1392	rBV	540223	1028486	12.53%	1.815%
13	13.417	1793	1800	1812	rBV	3753273	5907442	71.98%	10.422%
14	14.239	1934	1940	1946	rBV	905272	1367301	16.66%	2.412%
15	14.797	2028	2035	2046	rBV2	1045909	1698259	20.69%	2.996%
16	15.614	2170	2174	2182	rVB	60548	88310	1.08%	0.156%
17	16.290	2282	2289	2302	rBV	3540906	5489226	66.89%	9.685%
18	16.478	2317	2321	2332	rBV	85925	153199	1.87%	0.270%
19	17.277	2452	2457	2461	rBV	92811	111790	1.36%	0.197%
20	17.547	2496	2503	2511	rBV2	1318270	2135231	26.02%	3.767%
21	18.417	2646	2651	2660	rBV2	198228	314870	3.84%	0.556%
22	20.150	2940	2946	2952	rBV	6253558	8206673	100.00%	14.479%
23	21.472	3166	3171	3172	rBV5	79380	102072	1.24%	0.180%
24	21.854	3229	3236	3243	rBV2	1416734	2417704	29.46%	4.266%
25	23.581	3524	3530	3542	rVB2	112226	245520	2.99%	0.433%
26	25.232	3800	3811	3824	rBV	685949	2173363	26.48%	3.834%

Sum of corrected areas: 56680212

LSC Report - Integrated Chromatogram

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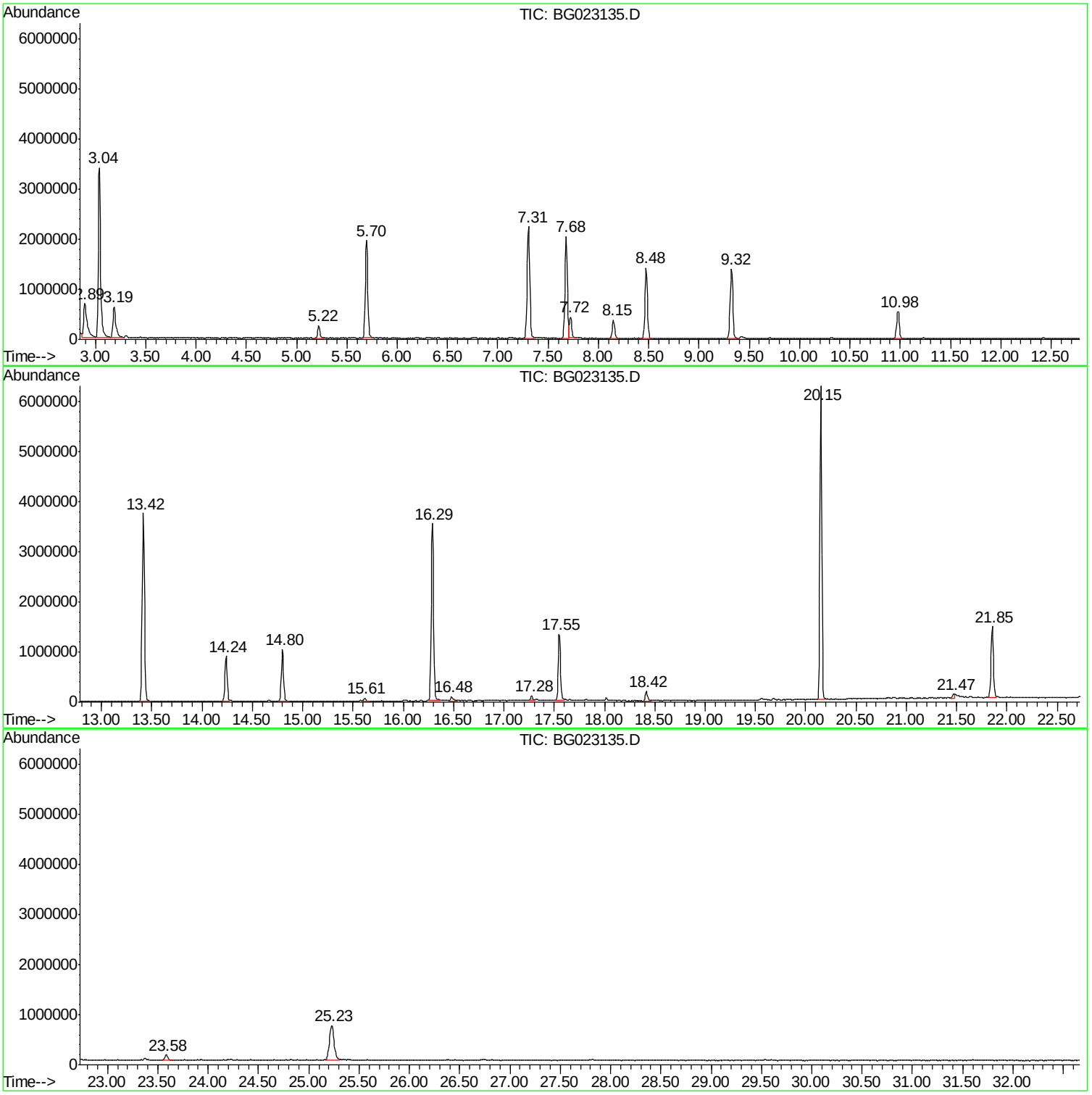
Operator : UM/SJ
Sample : H4015-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-22

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

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Instrument : BNA_G
ClientSampleId : C5-22

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

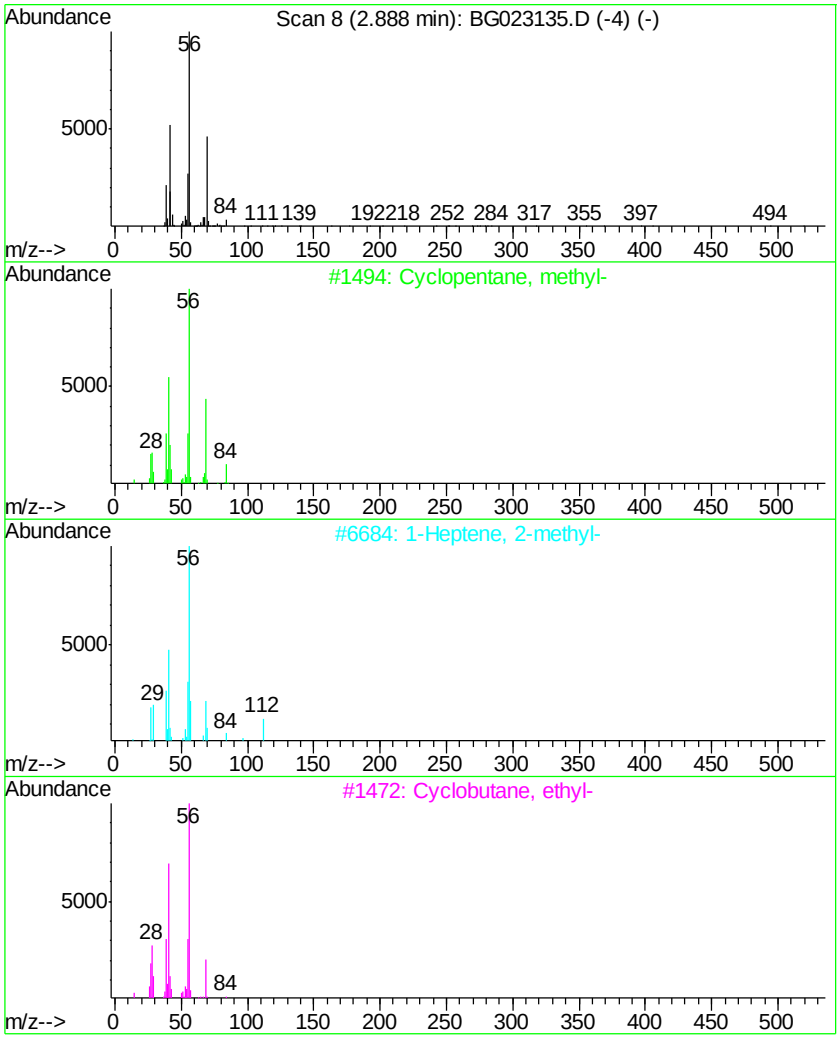
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

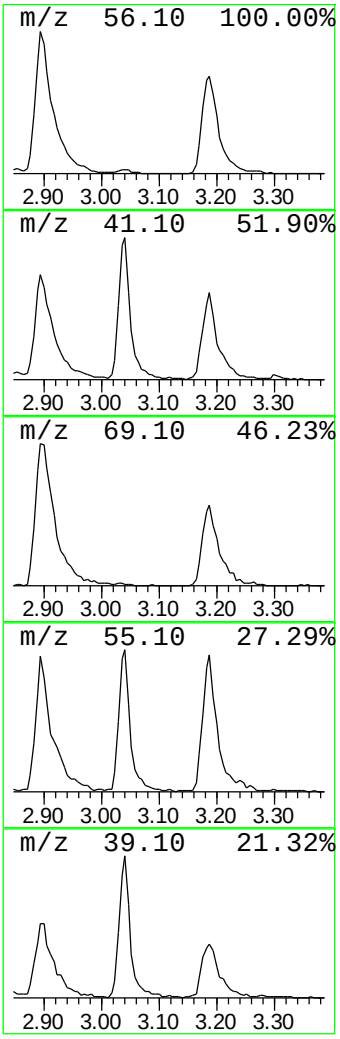
****

Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	48.40 ng	1566560	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	59





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Operator : UM/SJ
Sample : H4015-12
Misc :
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Instrument : BNA_G
ClientSampleId : C5-22

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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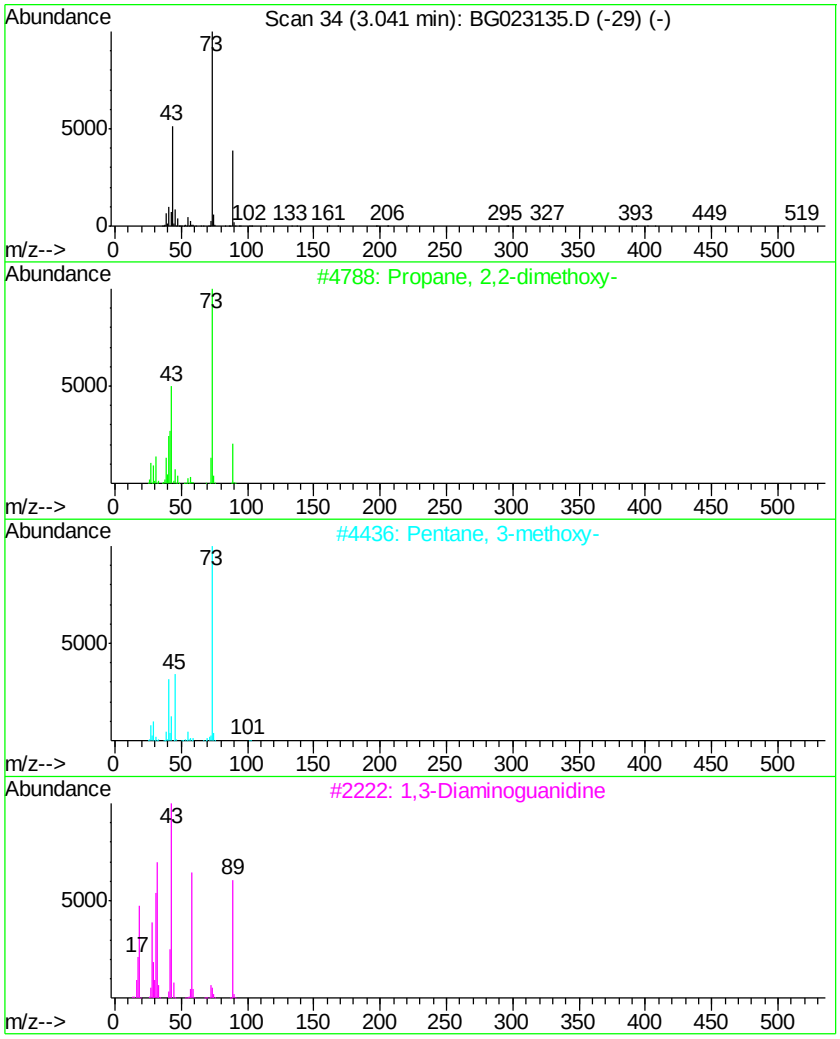
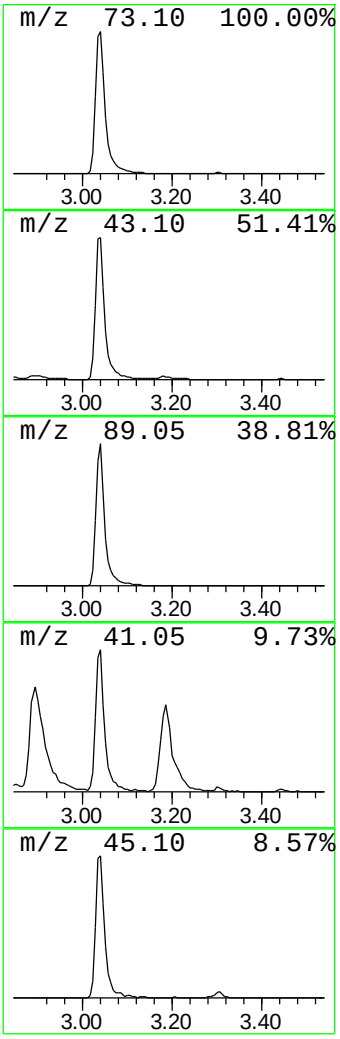
Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	156.51 ng	5066080	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	72
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023135.D
Acq On : 16 Jul 2016 6:57
Operator : UM/SJ
Sample : H4015-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C5-22

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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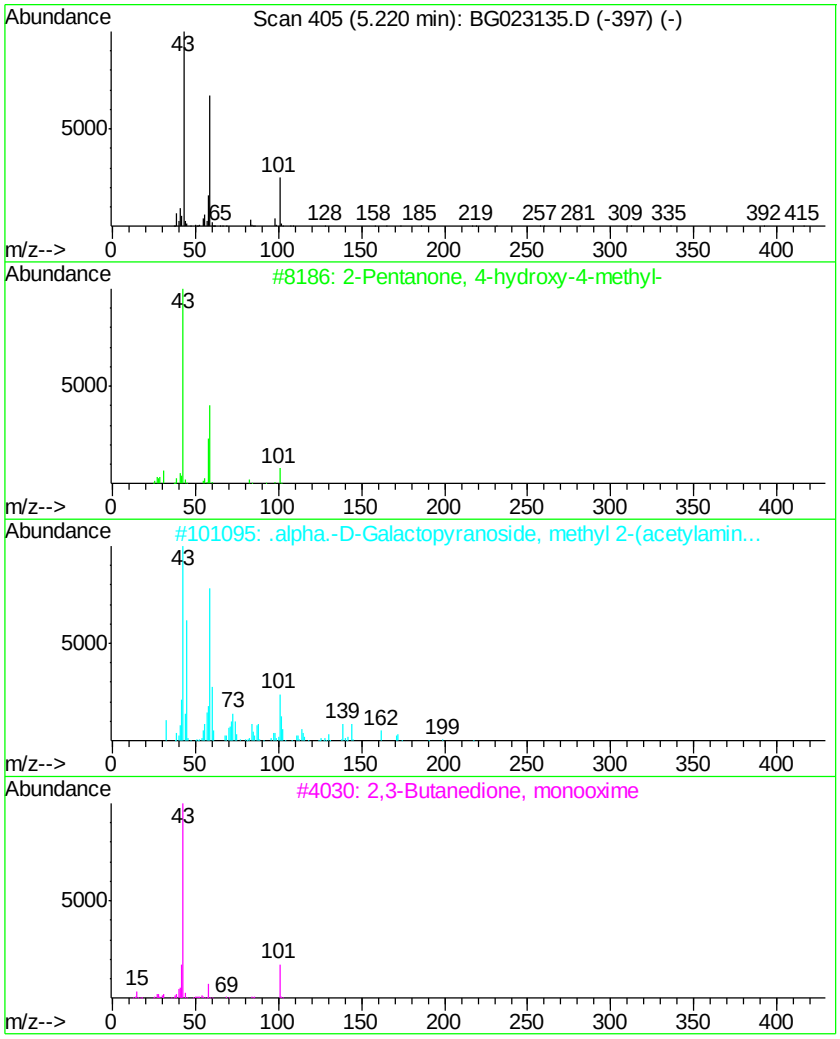
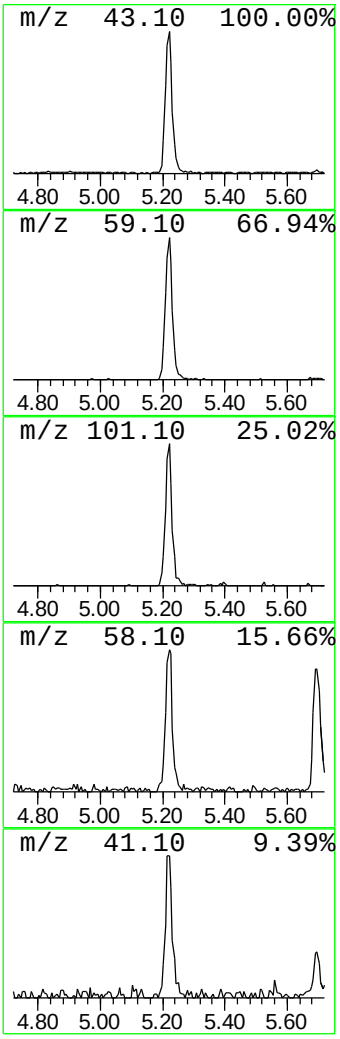
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	12.45 ng	403134	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	50
2	.alpha.-D-Galactopyranoside, met...	249	C10H19NO6	017296-07-0	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28
5	Acetamide	59	C2H5NO	000060-35-5	9





Library Search Compound Report

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Data File : BG023135.D
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Operator : UM/SJ
Sample : H4015-12
Misc :
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Instrument : BNA_G
ClientSampleId : C5-22

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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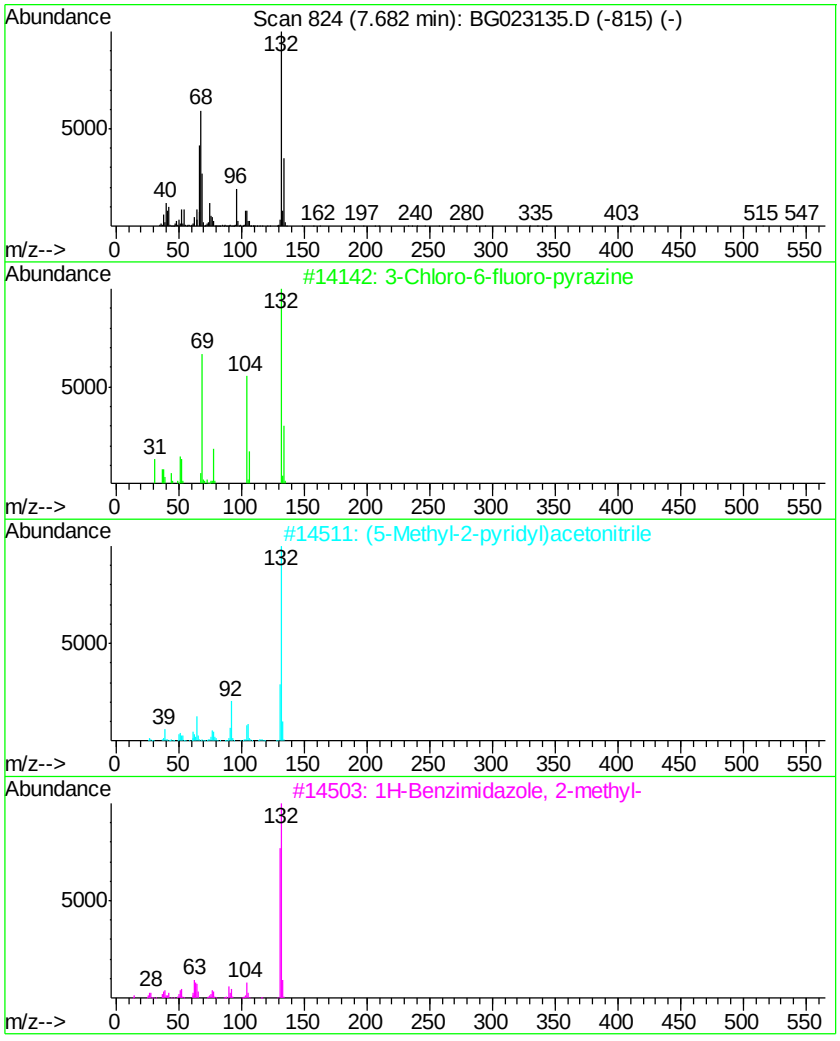
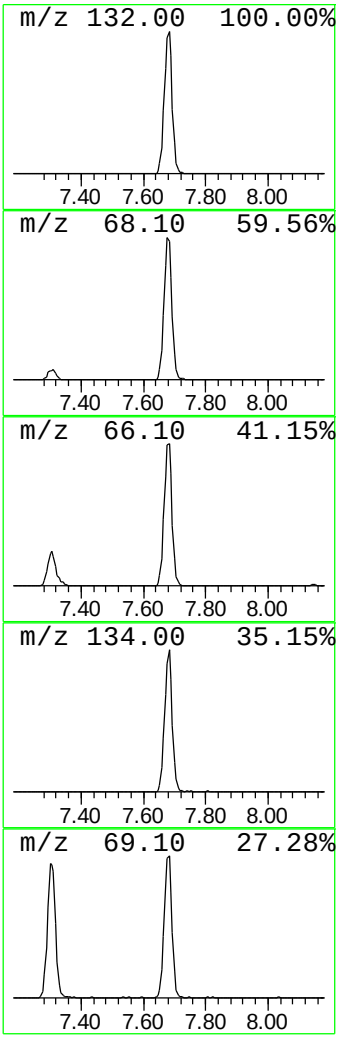
Peak Number 5 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	110.91 ng	3590050	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





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Sample : H4015-12
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Instrument : BNA_G
ClientSampleId : C5-22

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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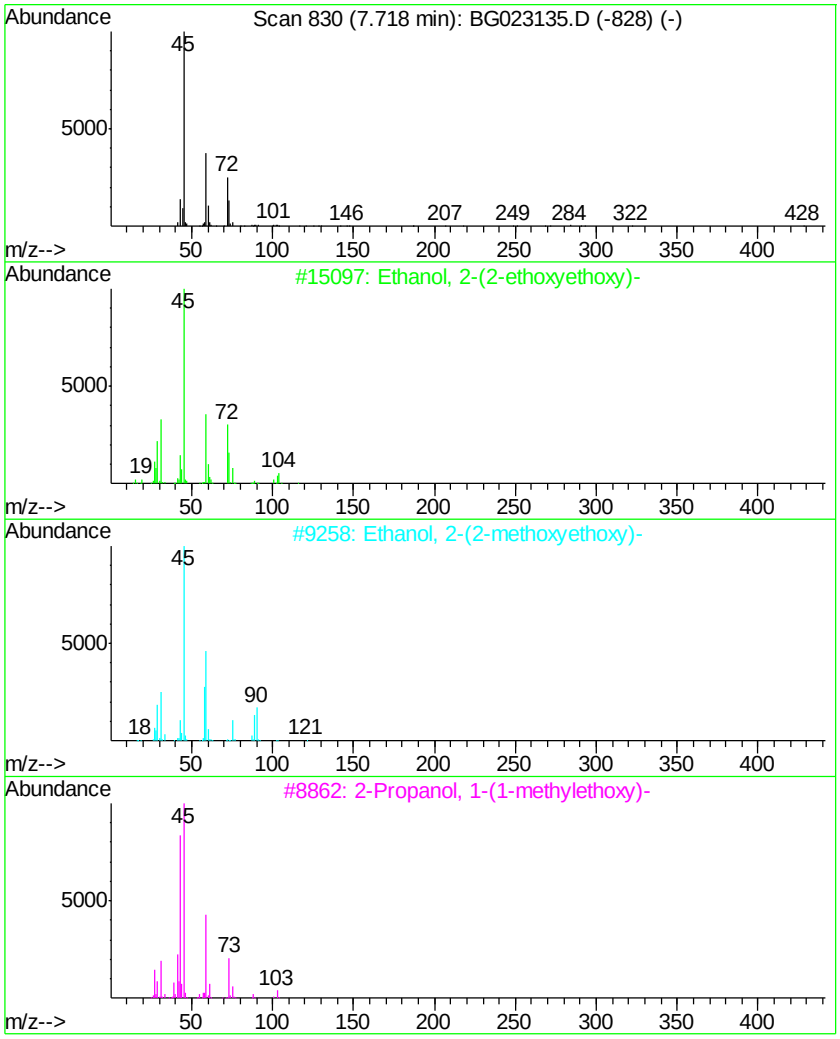
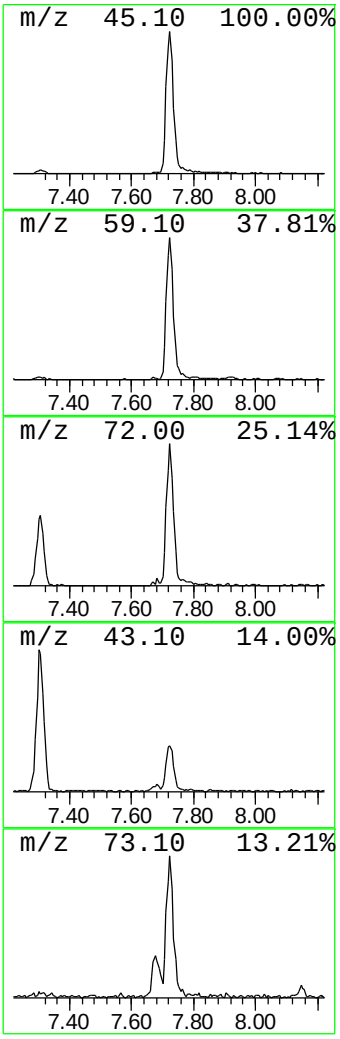
Peak Number 6 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	19.93 ng	645209	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	74
2	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	38
5	Methyl 2-(2-methoxyethoxy)acetate	148	C6H12O4	1000366-88-1	38





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Instrument : BNA_G
ClientSampleId : C5-22

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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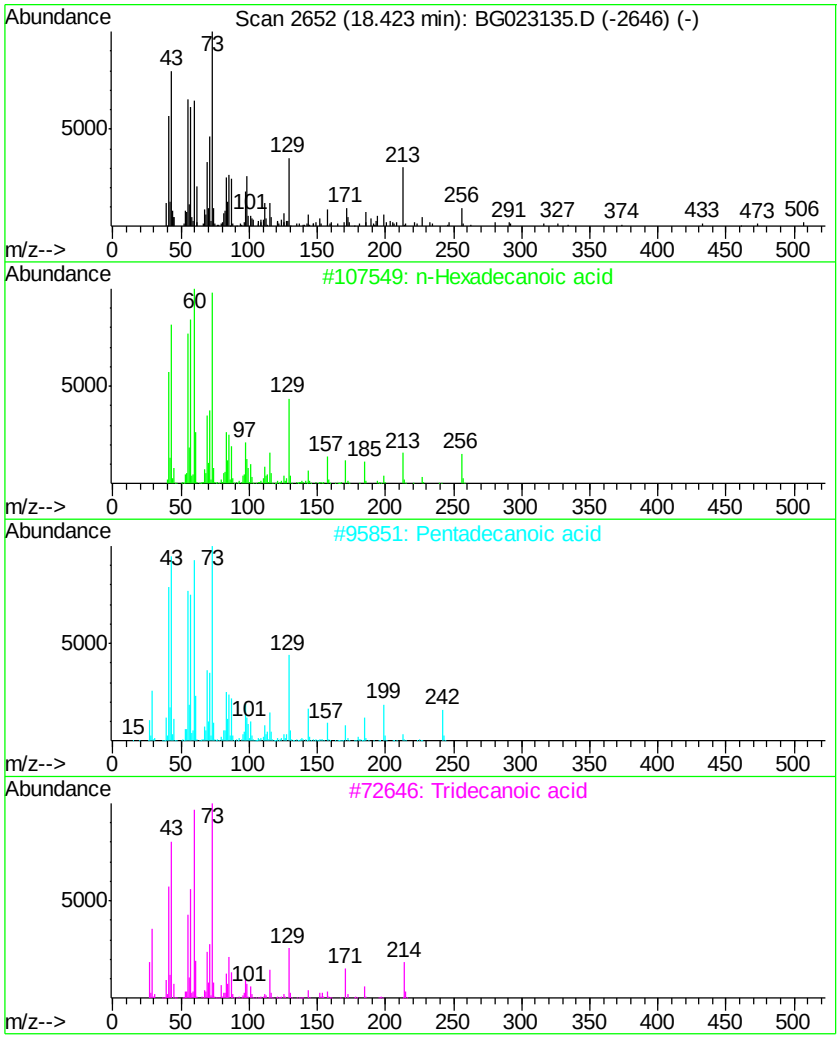
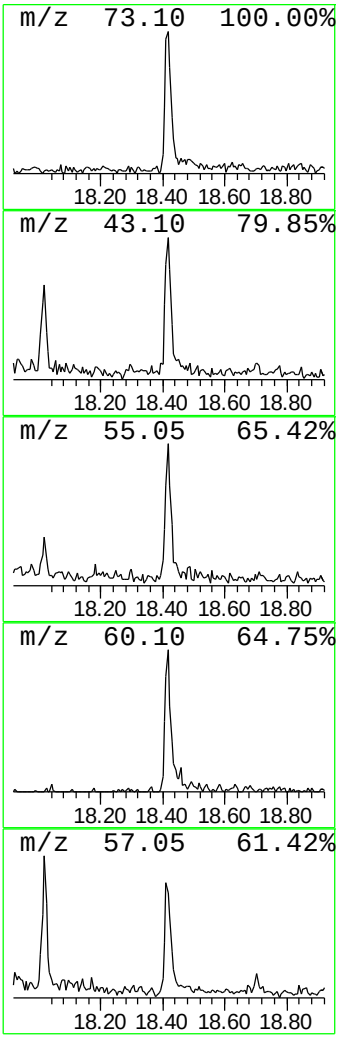
Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.95 ng	314870	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	n-Decanoic acid	172	C10H20O2	000334-48-5	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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

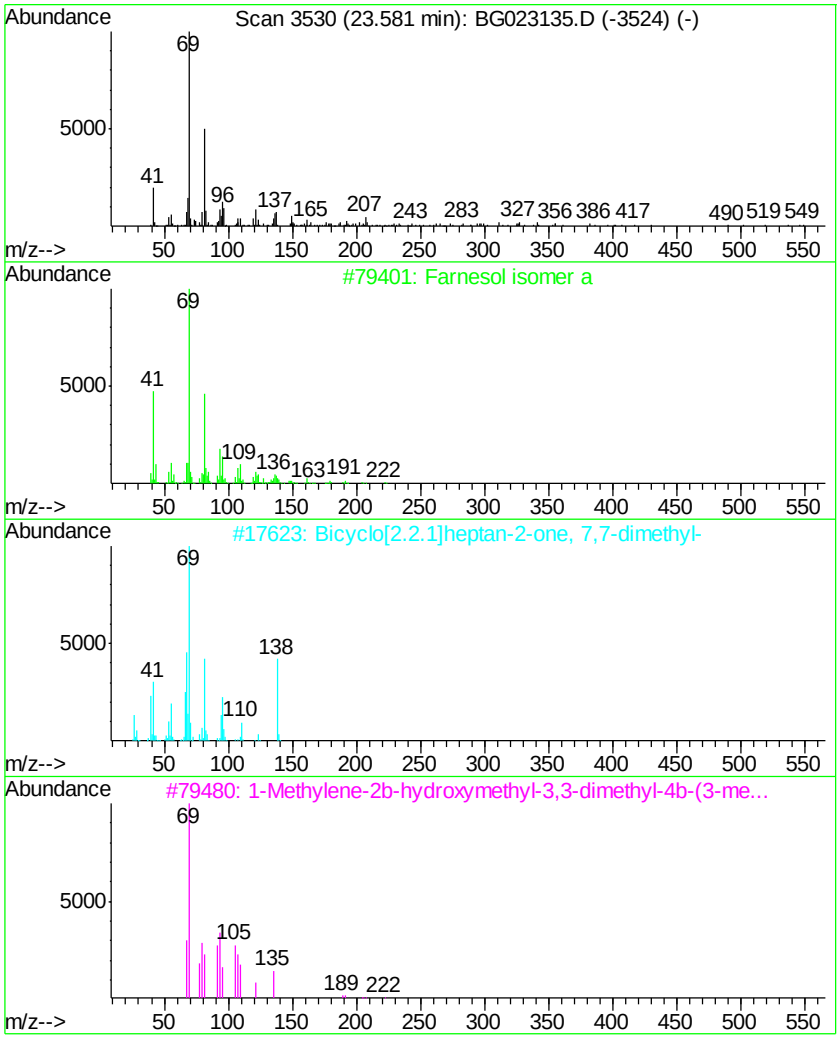
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

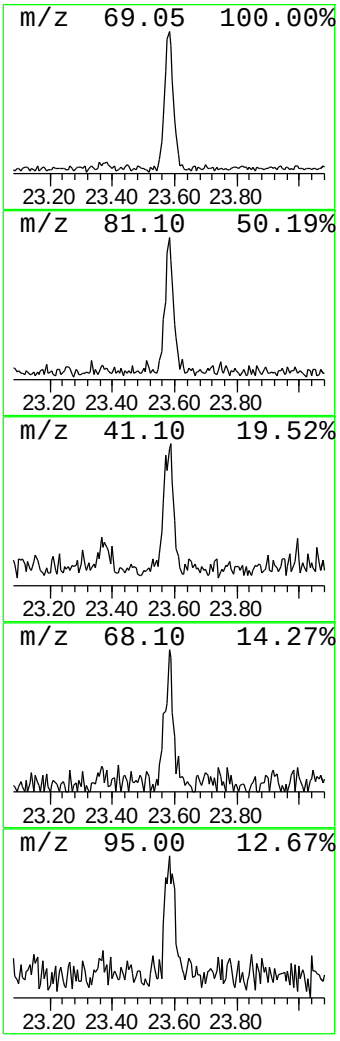
****

Peak Number 9 Farnesol isomer a Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	2.26 ng	245520	Perylene-d12	25.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	68
2	Bicyclo[2.2.1]heptan-2-one, 7,7-...	138	C9H14O	000514-15-8	64
3	1-Methylene-2b-hydroxymethyl-3,3...	222	C15H26O	1000144-10-6	59
4	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	59
5	1,3,5-Tris(cyanomethyl)-S-hexahy...	204	C9H12N6	004560-87-6	52





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, met...	2.89	48.4	ng	1566560	1	8.15	647394	20.0
Propane, 2,2-dime...	3.04	156.5	ng	5066080	1	8.15	647394	20.0
2-Pentanone, 4-hy...	5.22	12.4	ng	403134	1	8.15	647394	20.0
unknown7.68	7.68	110.9	ng	3590050	1	8.15	647394	20.0
Ethanol, 2-(2-eth...	7.72	19.9	ng	645209	1	8.15	647394	20.0
n-Hexadecanoic acid	18.42	3.0	ng	314870	4	17.55	2135230	20.0
Farnesol isomer a	23.58	2.3	ng	245520	6	25.23	2173360	20.0