LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024615.D
Acq On : 2 Nov 2016 6:22
Operator : UM/SJ
Sample : H5489-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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	19	24	36	rVB4	145797	417103	2.37%	0.552%
2	3.125	44	49	69	rVV	8983054	17622412	100.00%	23.338%
3	3.272	69	74	86	rVB4	169480	397805	2.26%	0.527%
4	4.718	313	320	329	rBV	259030	428302	2.43%	0.567%
5	5.329	415	424	435	rBV	1087454	1815040	10.30%	2.404%
6	5.799	495	504	512	rBV	2154444	3626880	20.58%	4.803%
7	7.403	769	777	789	rBV	2772062	5022281	28.50%	6.651%
8	7.791	835	843	855	rBV	2409624	4490308	25.48%	5.947%
9	8.267	917	924	931	rBV2	452780	819911	4.65%	1.086%
10	8.596	970	980	990	rBV	2031720	3673610	20.85%	4.865%
11	9.442	1115	1124	1134	rBV	1761537	3272904	18.57%	4.334%
12	11.093	1393	1405	1413	rBV	588995	1115354	6.33%	1.477%
13	13.507	1808	1816	1824	rBV	4287970	6832621	38.77%	9.049%
14	14.318	1948	1954	1961	rBV	1022417	1528772	8.68%	2.025%
15	14.882	2042	2050	2058	rBV2	983223	1551196	8.80%	2.054%
16	16.363	2295	2302	2310	rBV	1979429	3085049	17.51%	4.086%
17	17.626	2510	2517	2529	rBV2	1270343	2020199	11.46%	2.675%
18	20.205	2950	2956	2966	rBV	8430397	11736445	66.60%	15.543%
19	21.498	3171	3176	3183	rBV2	180101	333520	1.89%	0.442%
20	21.915	3240	3247	3255	rBV	1656672	2875093	16.31%	3.808%
21	25.352	3819	3832	3845	rBV2	902333	2845331	16.15%	3.768%

Sum of corrected areas: 75510136

LSC Report - Integrated Chromatogram

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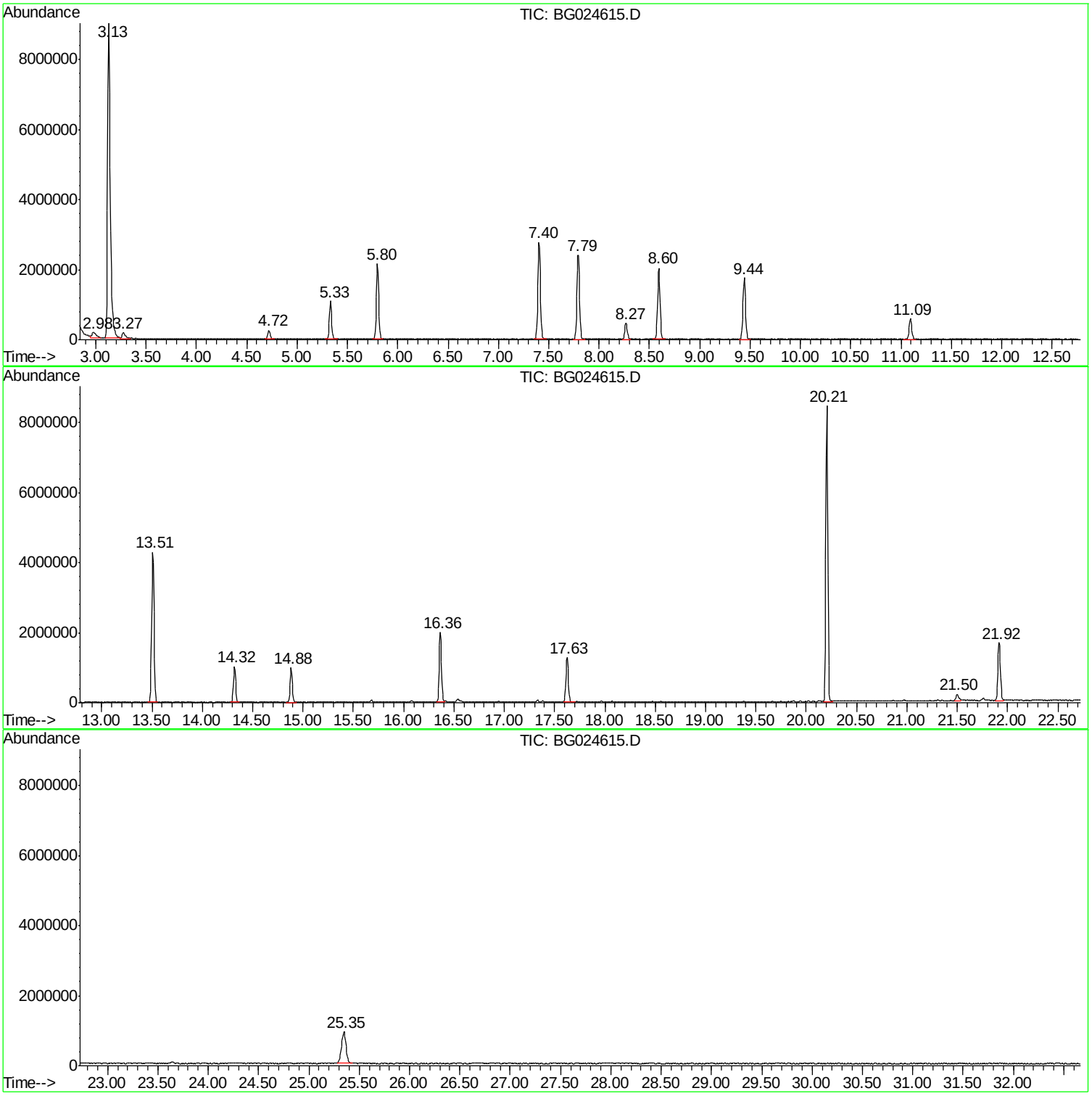
Operator : UM/SJ
Sample : H5489-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024615.D
Acq On : 2 Nov 2016 6:22
Operator : UM/SJ
Sample : H5489-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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

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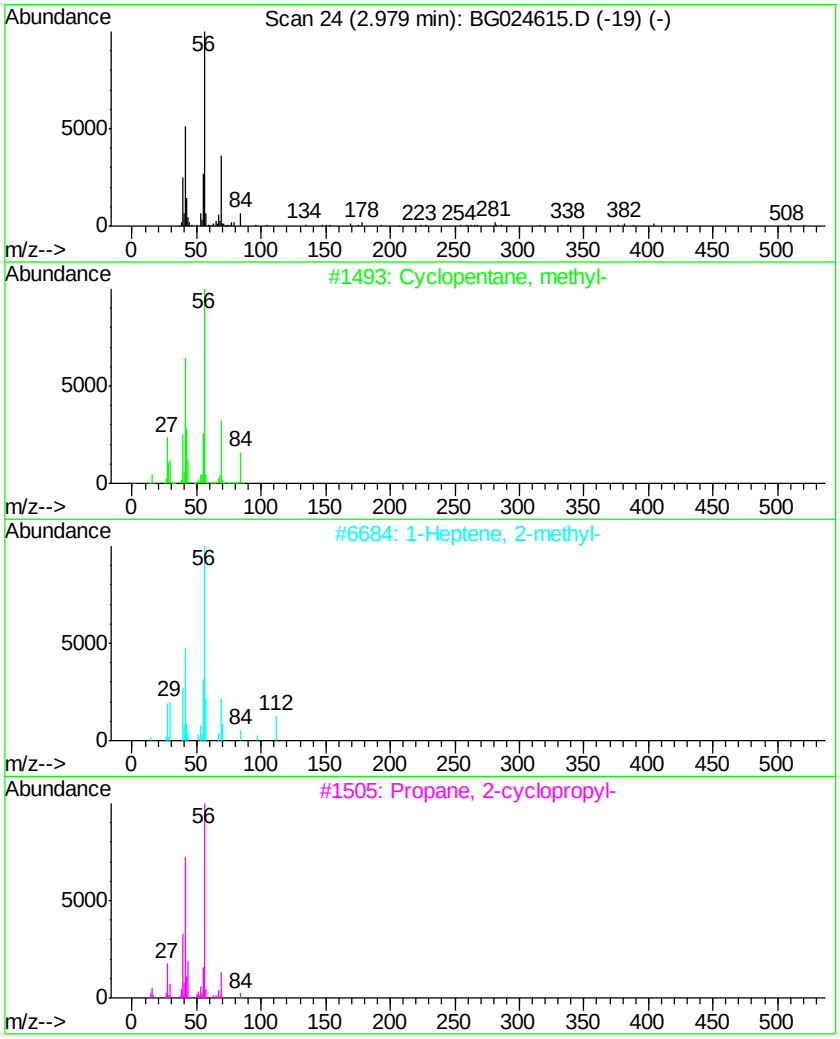
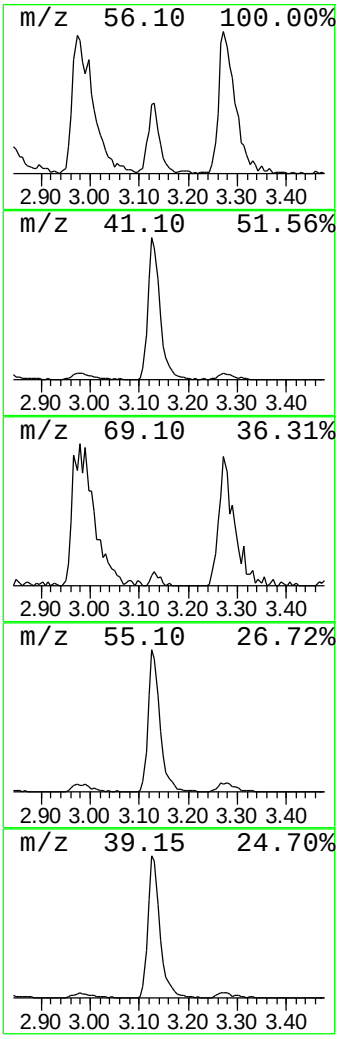
Peak Number 1 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	10.17 ng	417103	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
2	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	72
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	56
5	2-Methyl-1-nonene	140	C10H20	002980-71-4	56





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024615.D
Acq On : 2 Nov 2016 6:22
Operator : UM/SJ
Sample : H5489-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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

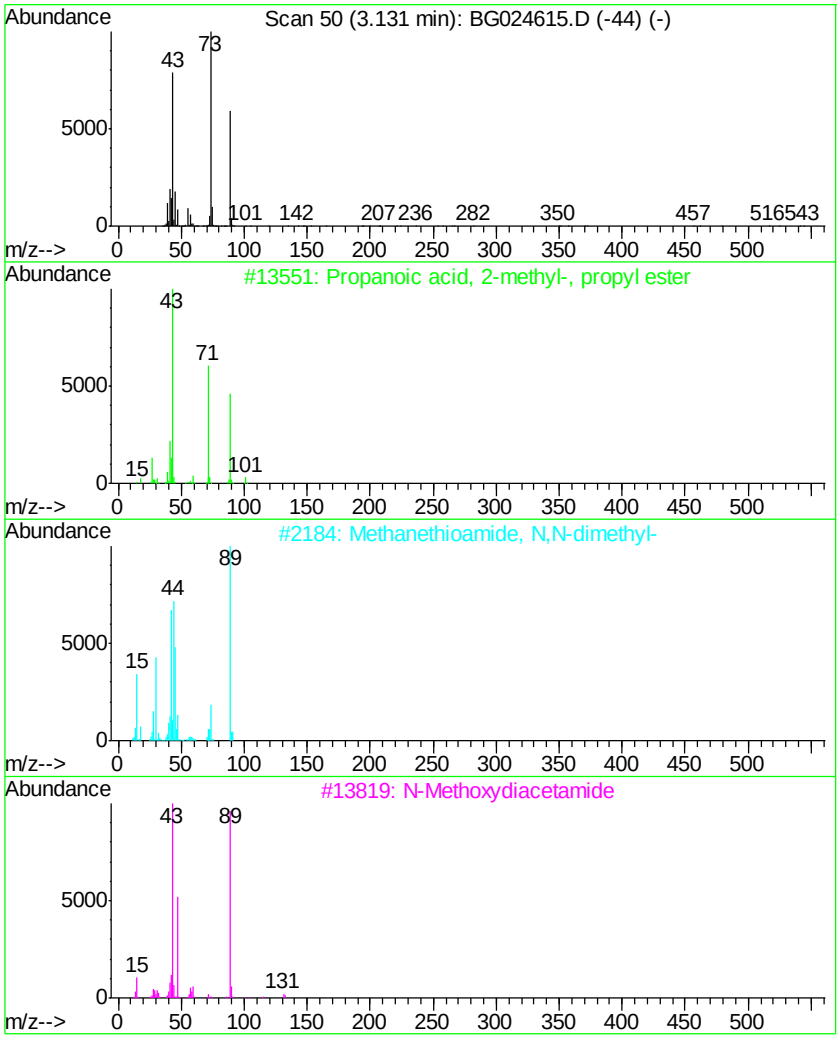
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

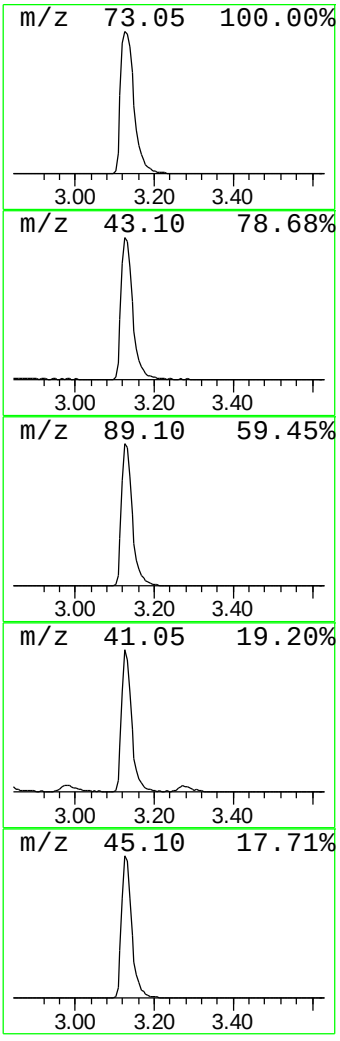
****

Peak Number 2 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	429.86 ng	17622400	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	47
2	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	37
3	N-Methoxydiacetamide	131	C5H9NO3	128459-09-6	28
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	23





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024615.D
Acq On : 2 Nov 2016 6:22
Operator : UM/SJ
Sample : H5489-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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

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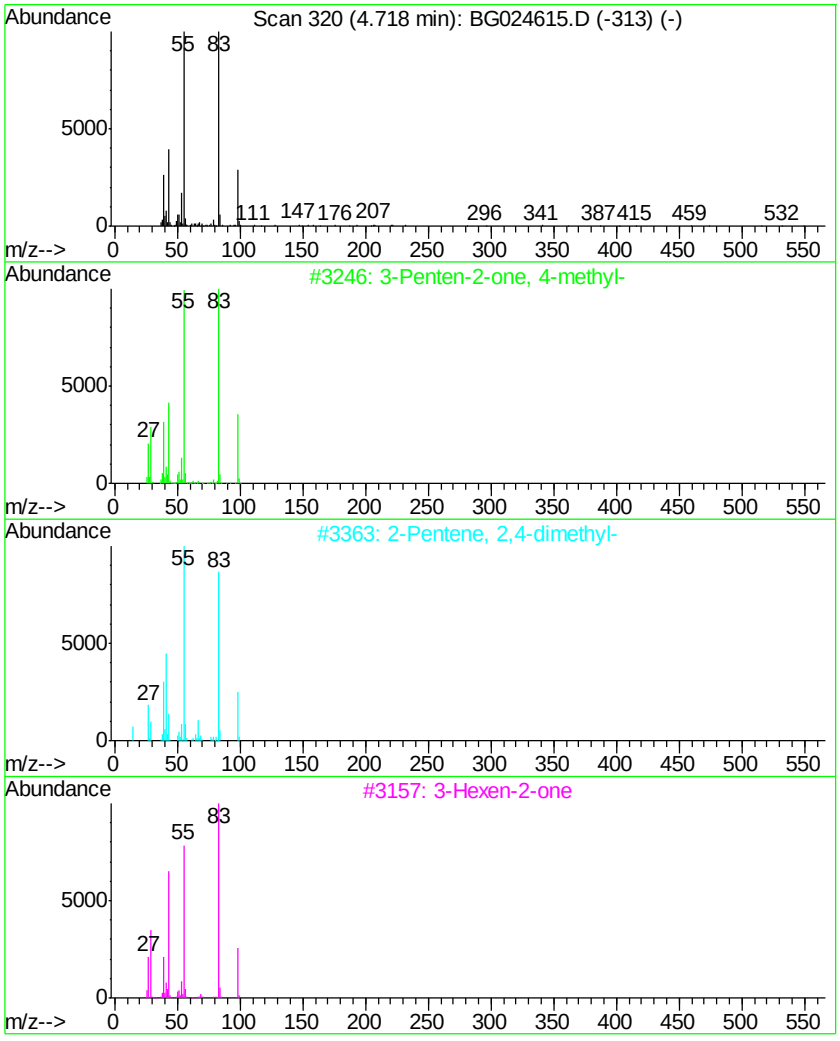
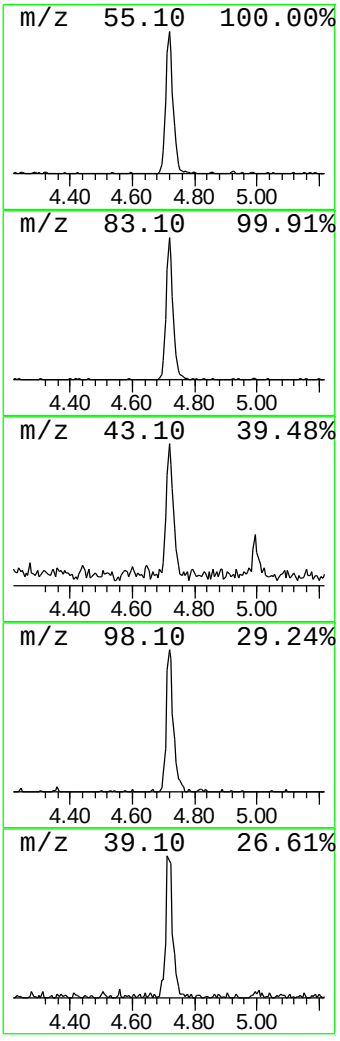
Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	10.45 ng	428302	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
3	3-Hexen-2-one	98	C6H10O	000763-93-9	86
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





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Sample : H5489-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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

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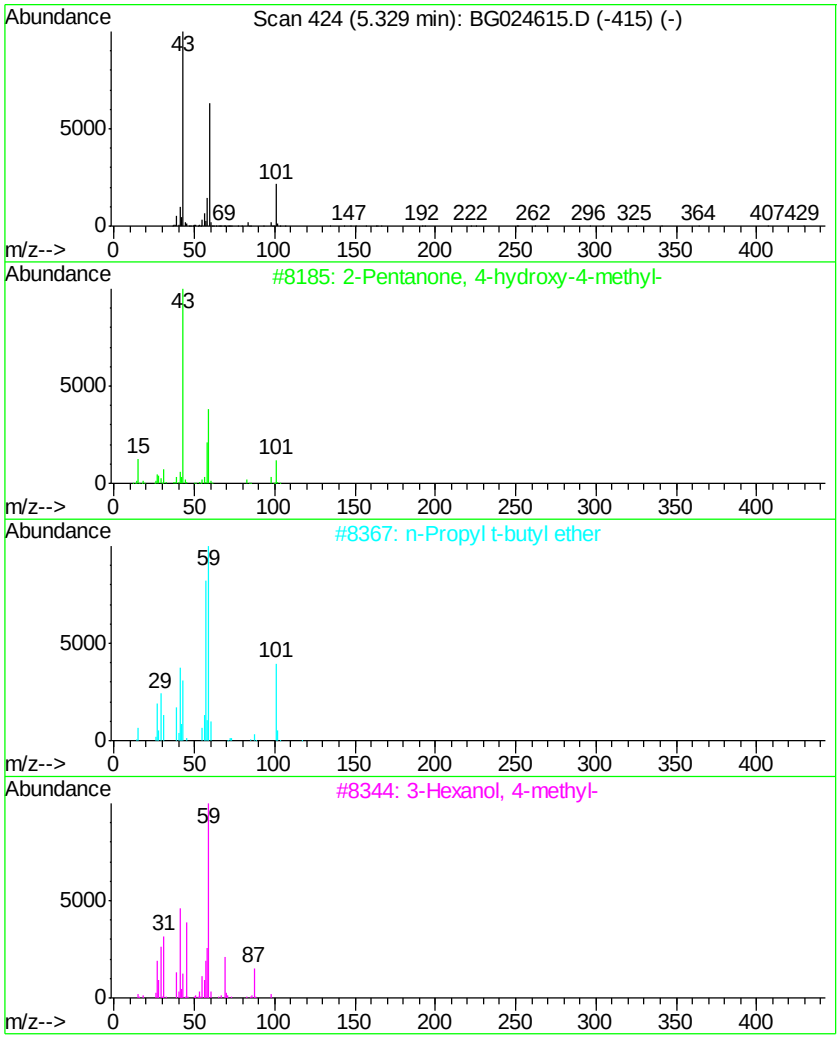
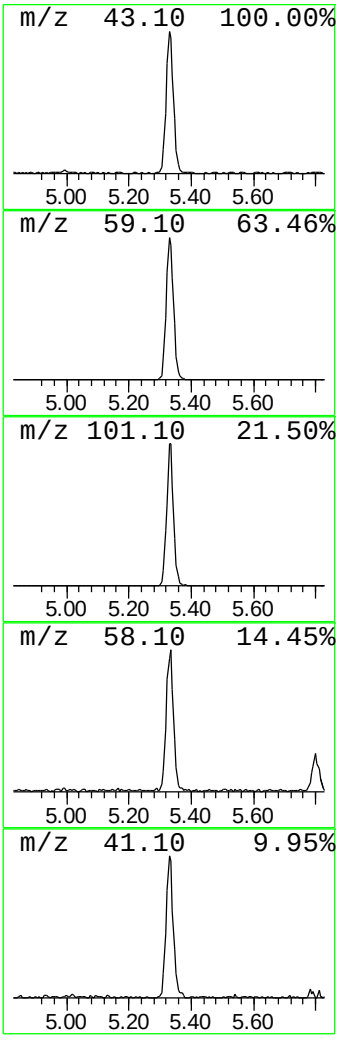
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	44.27 ng	1815040	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	56
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : H5489-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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

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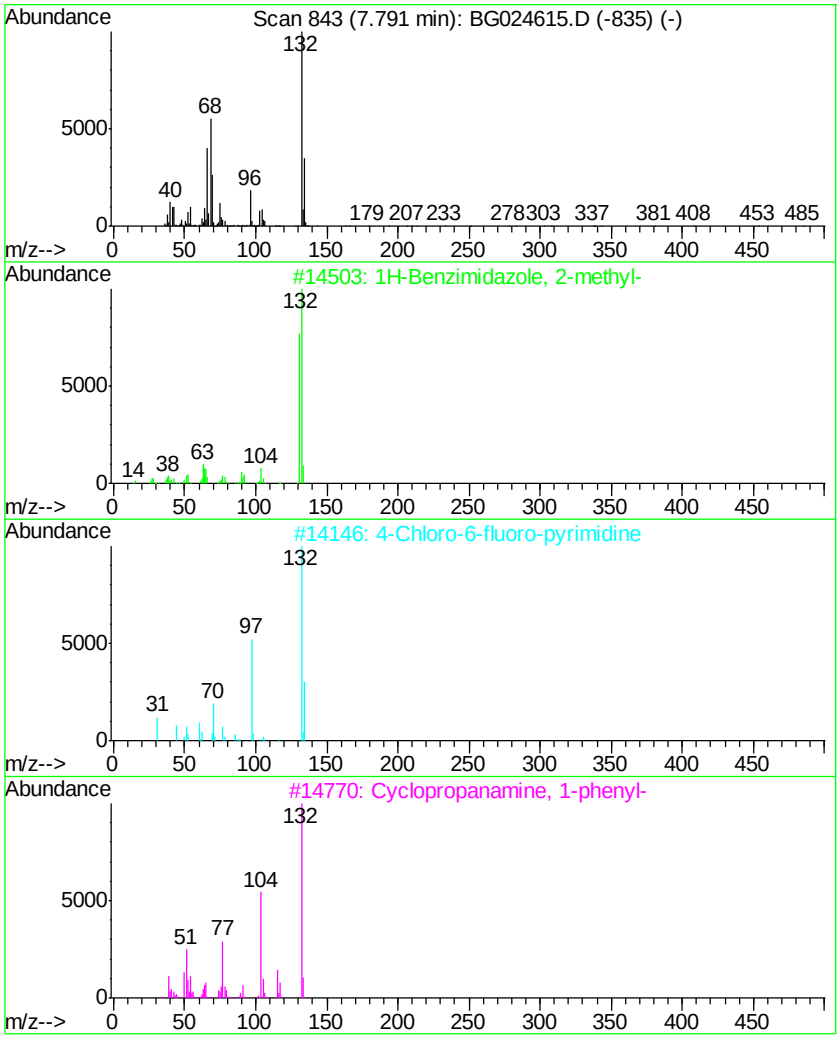
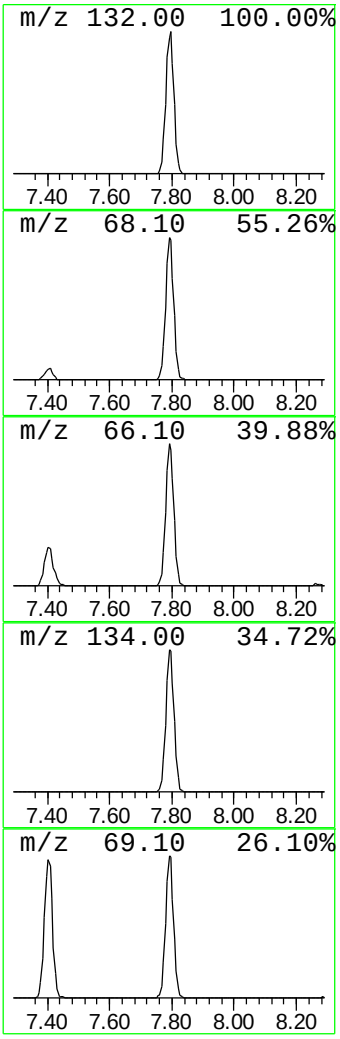
Peak Number 6 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	109.53 ng	4490310	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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Sample : H5489-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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

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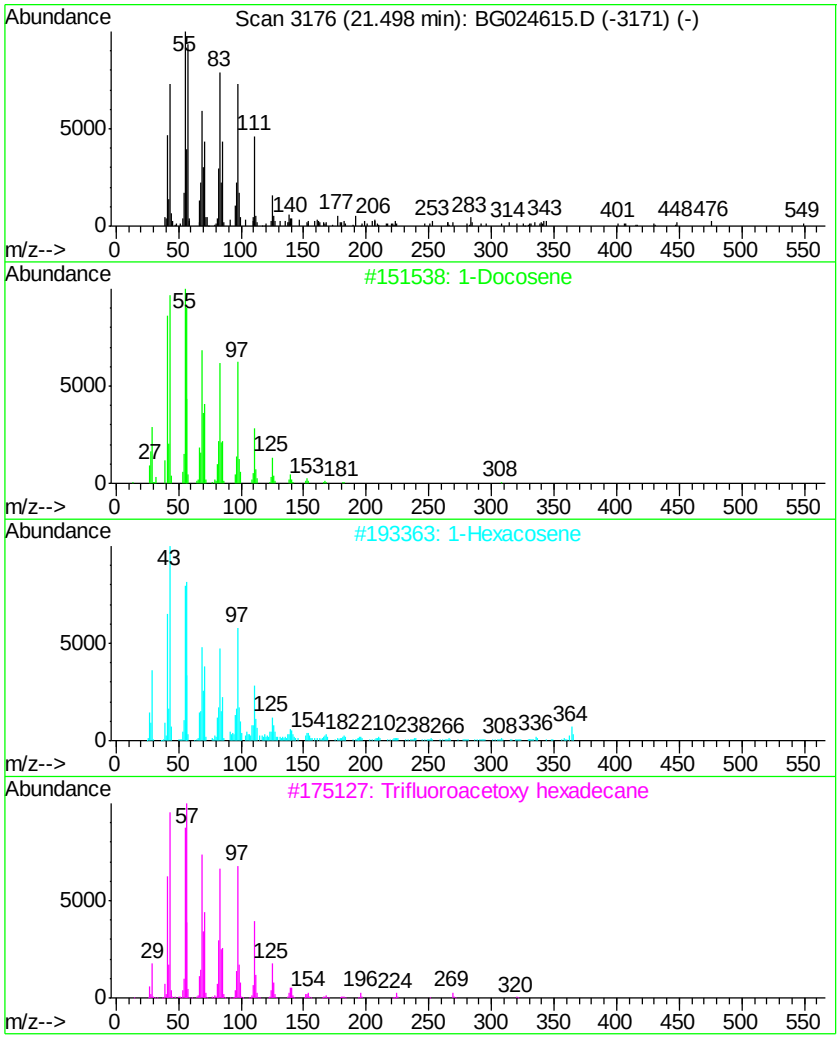
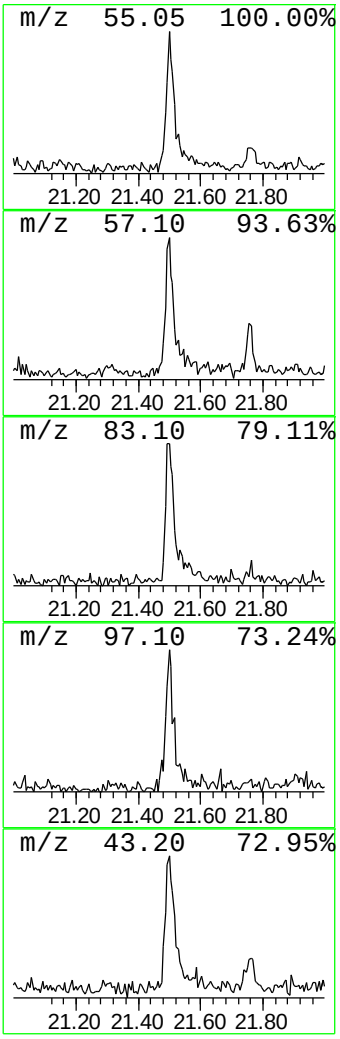
Peak Number 8 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	2.32 ng	333520	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	92
2	1-Hexacosene	364	C26H52	018835-33-1	87
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
4	Behenic alcohol	326	C22H46O	000661-19-8	87
5	Heneicosyl trifluoroacetate	408	C23H43F3O2	1000351-76-5	83





Tentatively Identified Compound (LSC) summary

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Operator : UM/SJ
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Instrument : BNA_G
ClientSampleId : SB-69-0.5-1.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, met...	2.98	10.2	ng	417103	1	8.27	819911	20.0
unknown3.13	3.13	429.9	ng	17622400	1	8.27	819911	20.0
3-Penten-2-one, 4...	4.72	10.4	ng	428302	1	8.27	819911	20.0
2-Pentanone, 4-hy...	5.33	44.3	ng	1815040	1	8.27	819911	20.0
unknown7.79	7.79	109.5	ng	4490310	1	8.27	819911	20.0
1-Docosene	21.50	2.3	ng	333520	5	21.92	2875090	20.0