LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024610.D
Acq On : 2 Nov 2016 3:09
Operator : UM/SJ
Sample : H5489-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73-13.5-14.0

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	3.131	44	50	69	rVB	9012266	19695539	100.00%	24.109%
2	5.334	416	425	433	rBV	622289	985511	5.00%	1.206%
3	5.804	497	505	516	rBV	2731327	4779364	24.27%	5.850%
4	7.408	768	778	788	rBV	2938037	5341348	27.12%	6.538%
5	7.796	835	844	853	rBV	2788355	4946350	25.11%	6.055%
6	8.272	916	925	932	rBV	452987	833993	4.23%	1.021%
7	8.595	972	980	993	rBV	2107944	3829302	19.44%	4.687%
8	9.447	1117	1125	1133	rBV	1799526	3327665	16.90%	4.073%
9	11.098	1395	1406	1414	rBV	630702	1134187	5.76%	1.388%
10	13.513	1807	1817	1825	rVB	4546056	7175023	36.43%	8.783%
11	14.323	1947	1955	1962	rBV	1099205	1624952	8.25%	1.989%
12	14.887	2044	2051	2058	rVB	969269	1565425	7.95%	1.916%
13	16.368	2295	2303	2312	rBV	4290871	6537190	33.19%	8.002%
14	17.625	2511	2517	2525	rVB	1276640	1981087	10.06%	2.425%
15	18.472	2657	2661	2667	rBV3	137957	204507	1.04%	0.250%
16	20.211	2950	2957	2963	rBV	7929894	11106298	56.39%	13.595%
17	20.980	3076	3088	3091	rBV4	177296	529626	2.69%	0.648%
18	21.503	3172	3177	3185	rBV3	252712	489736	2.49%	0.599%
19	21.920	3240	3248	3262	rVB	1607193	2831496	14.38%	3.466%
20	25.358	3819	3833	3847	rBV3	843269	2774169	14.09%	3.396%

Sum of corrected areas: 81692768

LSC Report - Integrated Chromatogram

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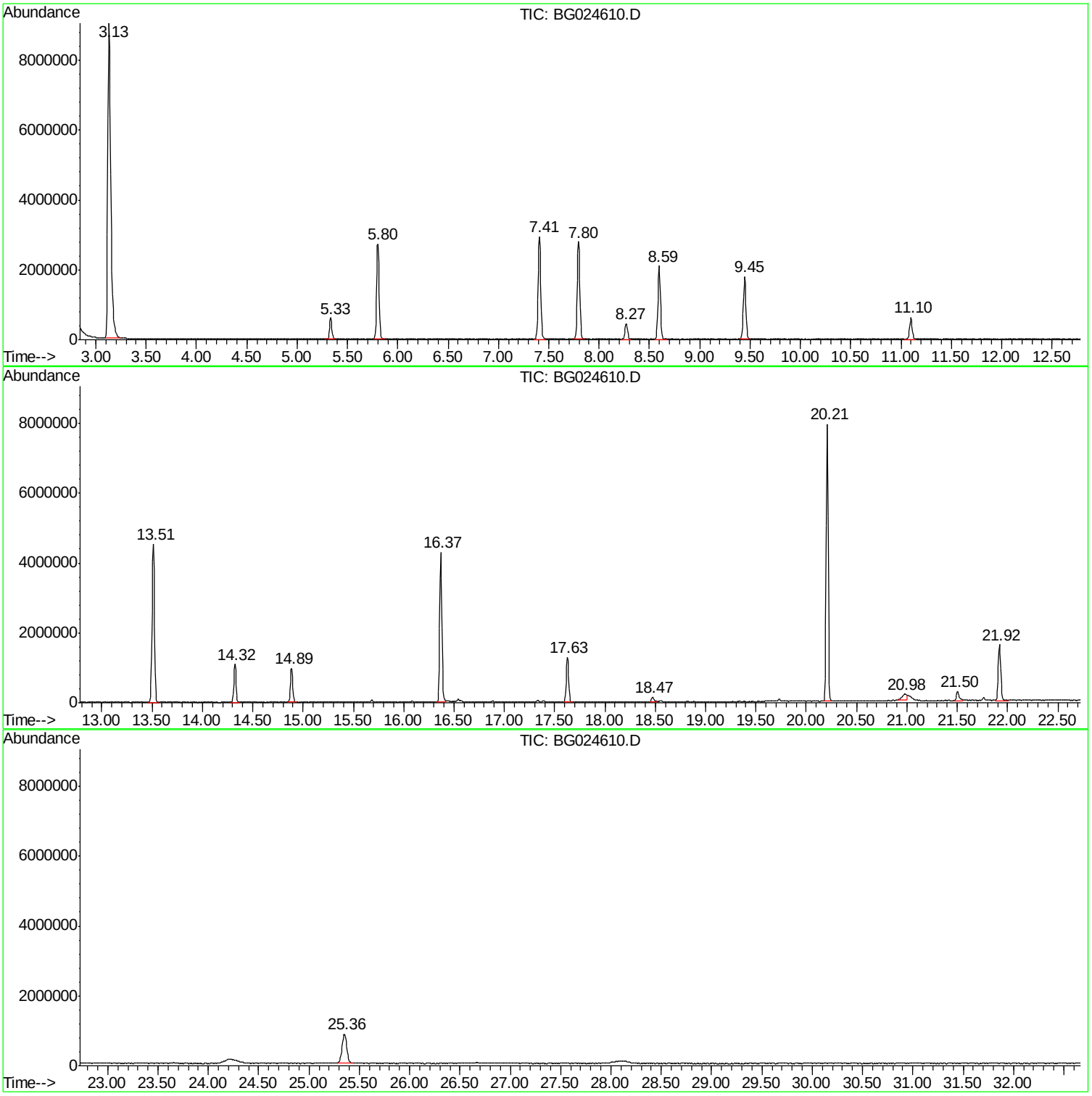
Sample : H5489-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73-13.5-14.0

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 : BG024610.D
Acq On : 2 Nov 2016 3:09
Operator : UM/SJ
Sample : H5489-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73-13.5-14.0

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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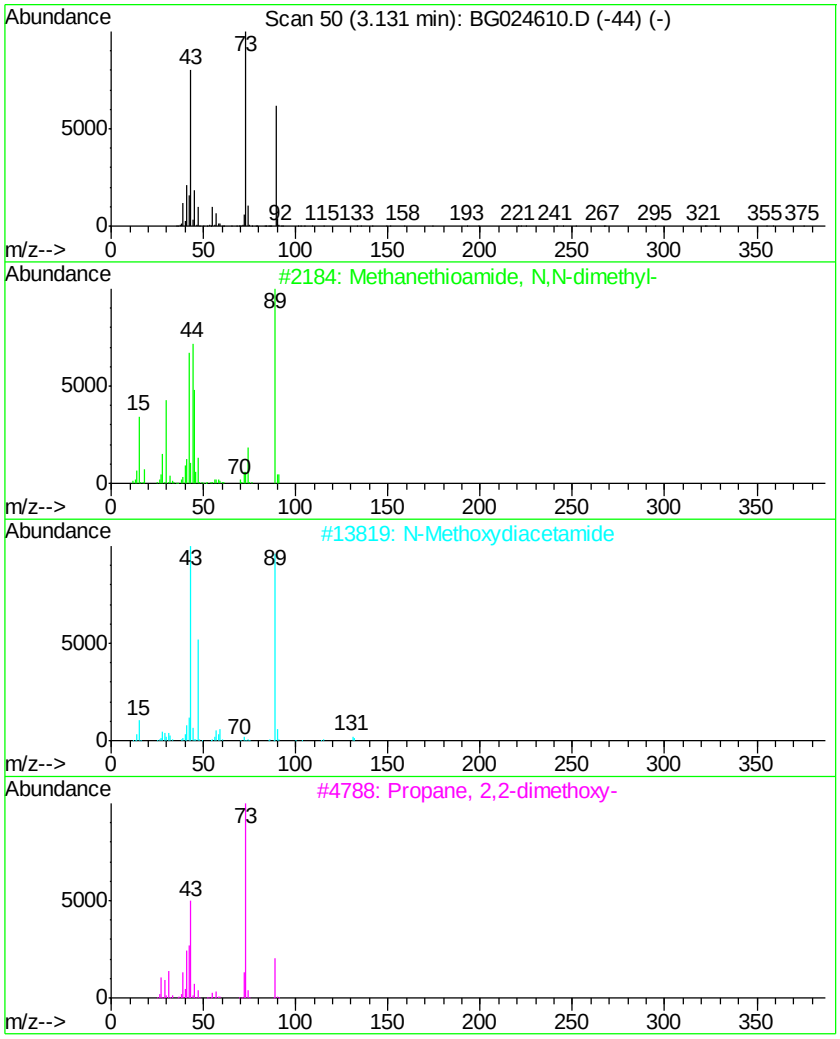
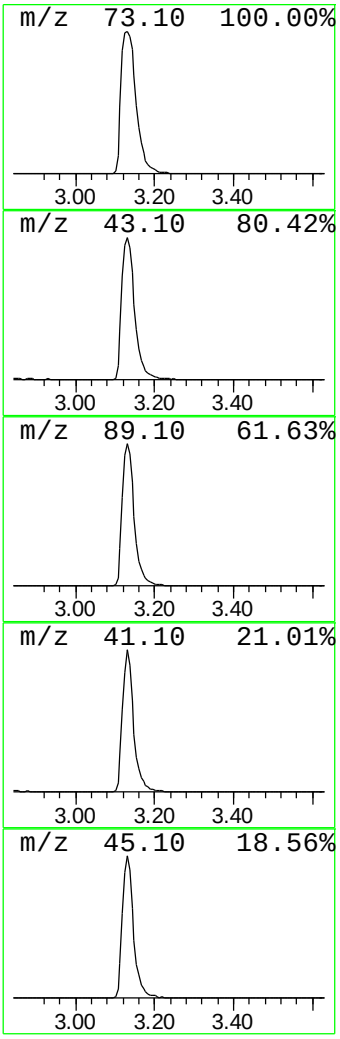
Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	472.32 ng	19695500	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	37
2	N-Methoxydiacetamide	131	C5H9NO3	128459-09-6	25
3	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	23
4	1-Hepten-4-ol	114	C7H14O	003521-91-3	17
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	16





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024610.D
Acq On : 2 Nov 2016 3:09
Operator : UM/SJ
Sample : H5489-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73-13.5-14.0

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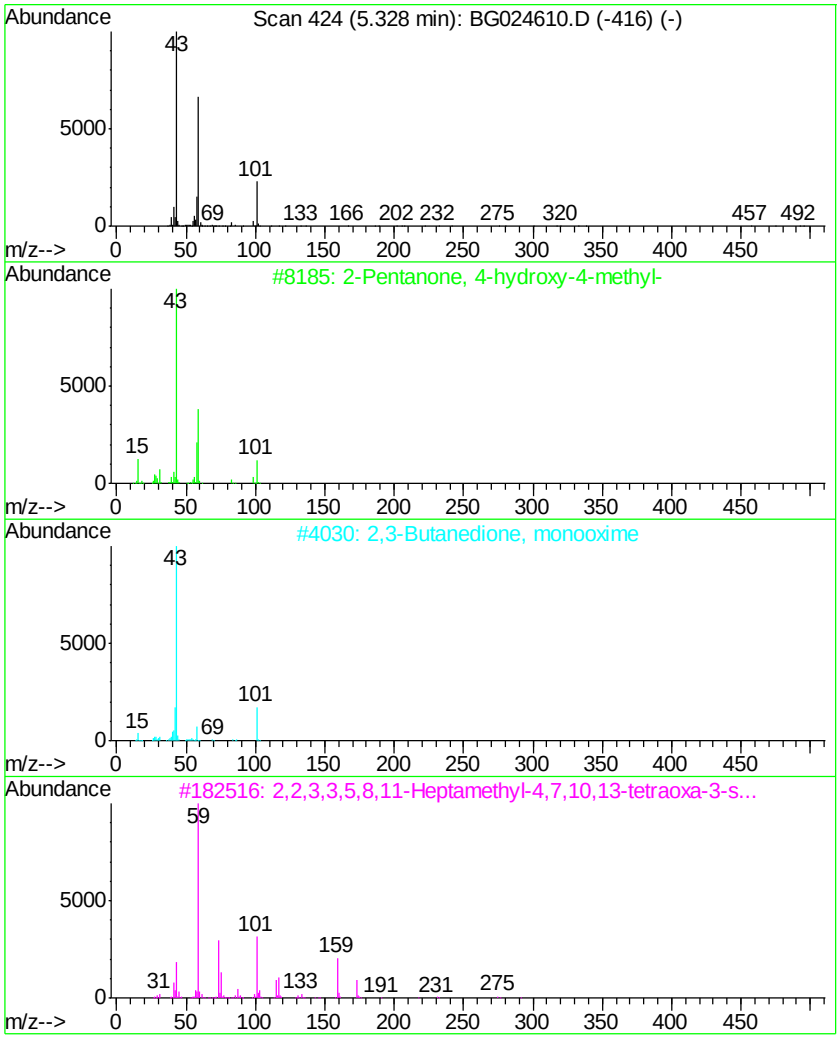
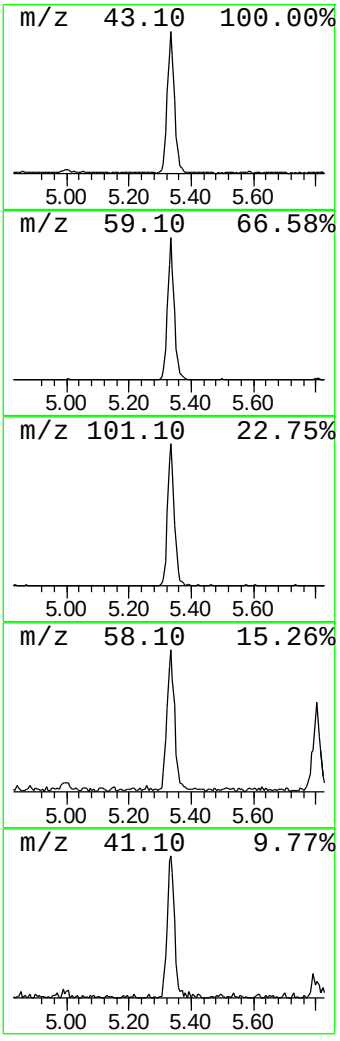
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	23.63 ng	985511	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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	2,2,3,3,5,8,11-Heptamethyl-4,7,1...	348	C18H40O4Si	1000367-07-2	28
4	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024610.D
Acq On : 2 Nov 2016 3:09
Operator : UM/SJ
Sample : H5489-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73-13.5-14.0

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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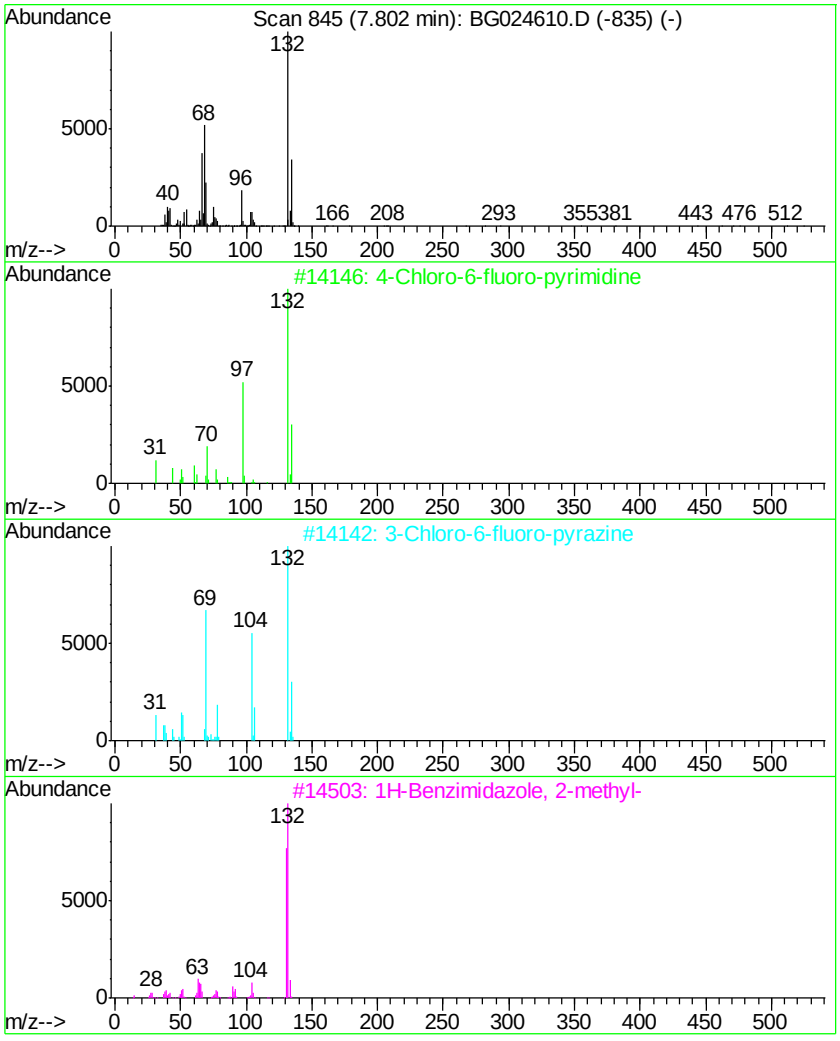
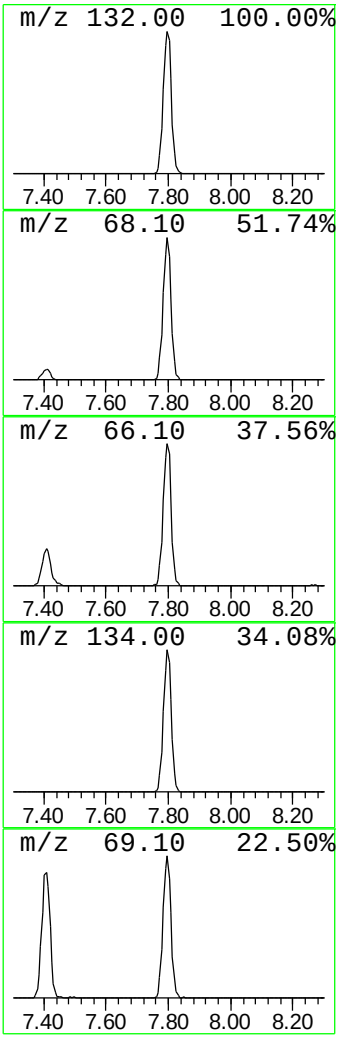
Peak Number 3 unknown7.80 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.80	118.62 ng	4946350	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	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
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Operator : UM/SJ
Sample : H5489-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73-13.5-14.0

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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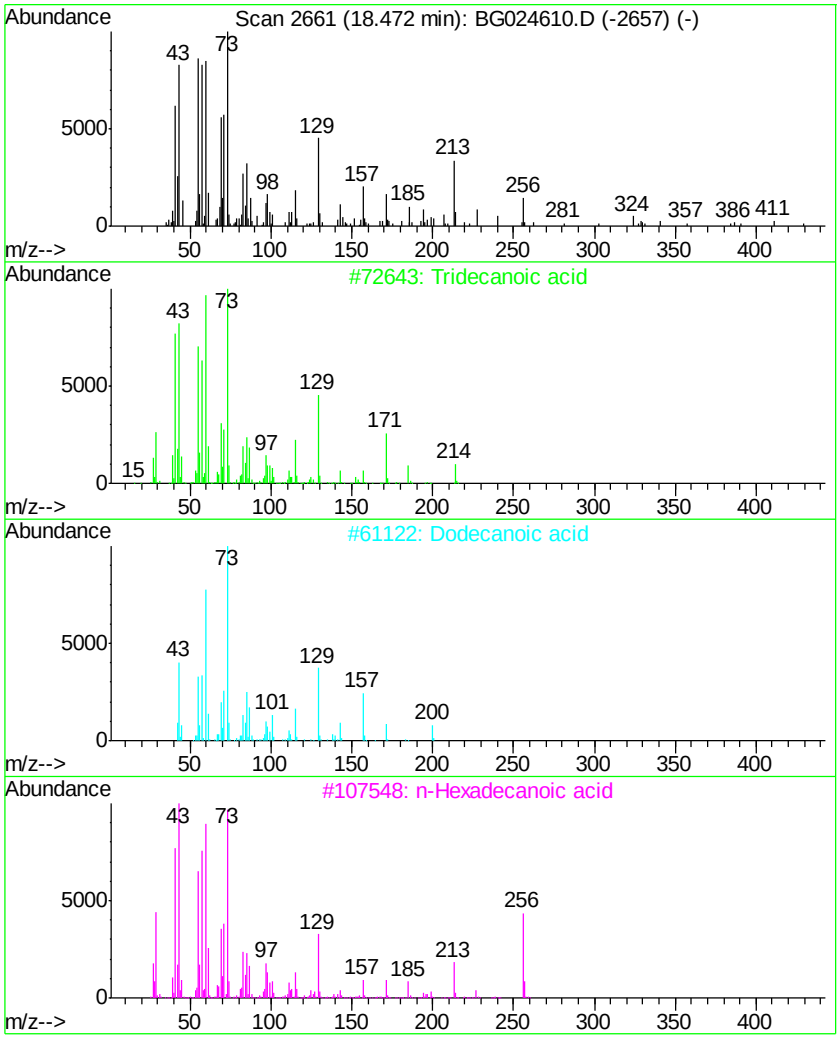
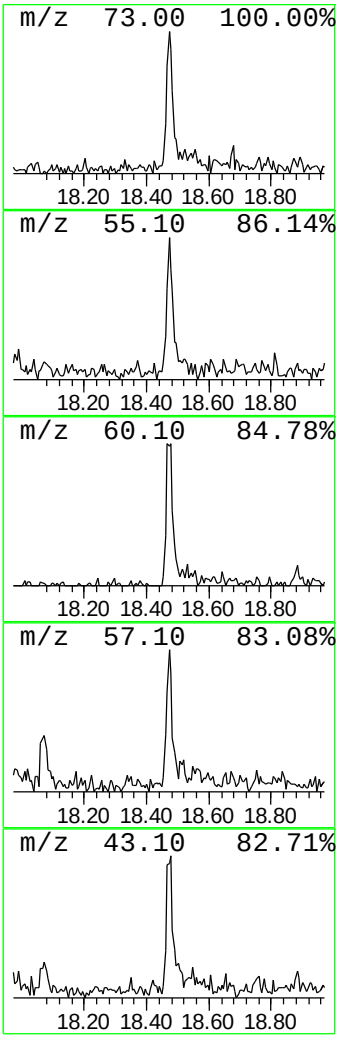
Peak Number 5 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.06 ng	204507	Phenanthrene-d10	17.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	89
2	Dodecanoic acid	200	C12H24O2	000143-07-7	72
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110116\
Data File : BG024610.D
Acq On : 2 Nov 2016 3:09
Operator : UM/SJ
Sample : H5489-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73-13.5-14.0

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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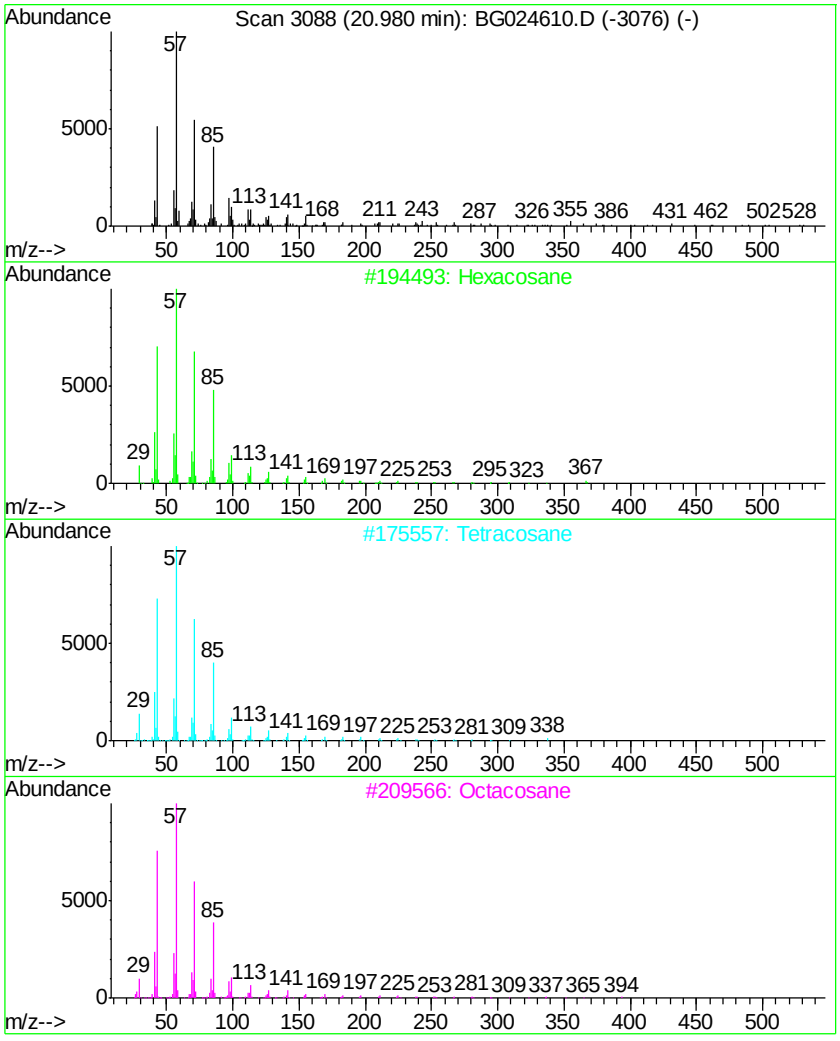
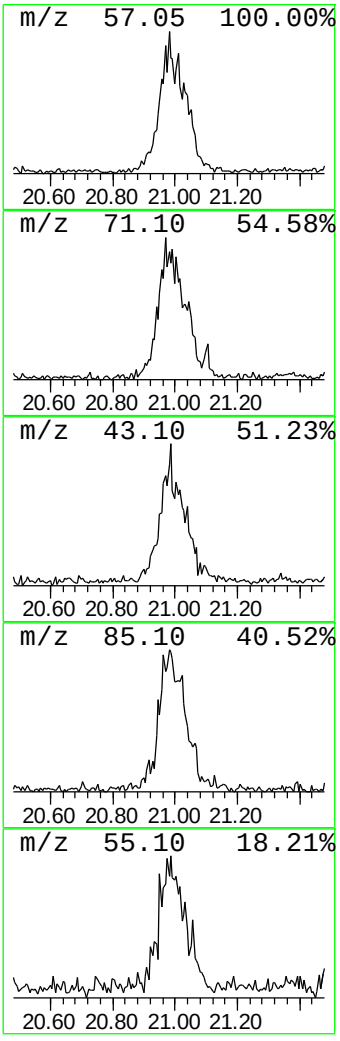
Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.98	3.74 ng	529626	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Tetracosane	338	C24H50	000646-31-1	83
3	Octacosane	394	C28H58	000630-02-4	83
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	83
5	Eicosane	282	C20H42	000112-95-8	81





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Operator : UM/SJ
Sample : H5489-13
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-73-13.5-14.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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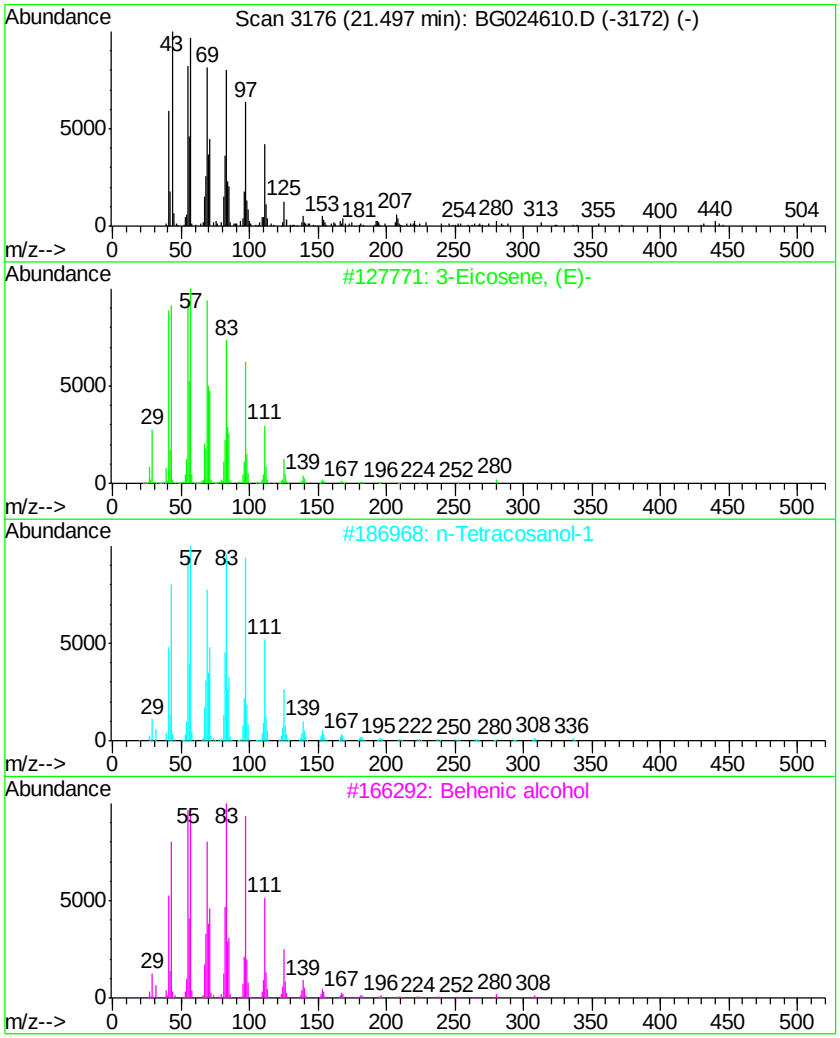
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

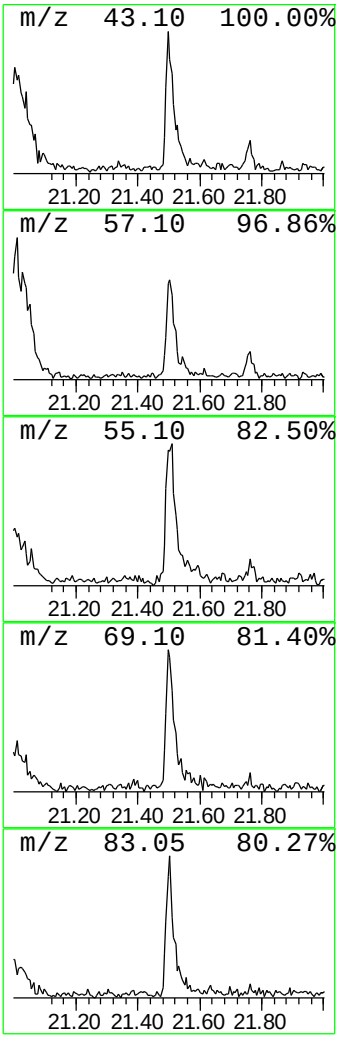
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	3.46 ng	489736	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	97
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	90
5	Cycloeicosane	280	C20H40	000296-56-0	89





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
unknown3.13	3.13	472.3	ng	19695500	1	8.27	833993	20.0
2-Pentanone, 4-hy...	5.33	23.6	ng	985511	1	8.27	833993	20.0
unknown7.80	7.80	118.6	ng	4946350	1	8.27	833993	20.0
Tridecanoic acid	18.47	2.1	ng	204507	4	17.63	1981090	20.0
Hexacosane	20.98	3.7	ng	529626	5	21.92	2831500	20.0
3-Eicosene, (E)-	21.50	3.5	ng	489736	5	21.92	2831500	20.0