LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083829.D
Acq On : 15 Dec 2015 22:35
Operator : UM/IZ
Sample : G4782-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-D-B

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_F\METHODS\8270-BF121315.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	4.441	203	206	210	rVB	69751	82709	3.32%	0.546%
2	5.081	259	262	264	rBV	445145	448604	17.98%	2.959%
3	5.504	297	299	302	rBV	822124	727672	29.17%	4.799%
4	5.904	332	334	337	rVB	64009	57971	2.32%	0.382%
5	6.521	386	388	391	rBV	349997	480869	19.28%	3.172%
6	6.670	398	401	403	rBV	1518036	1356581	54.38%	8.947%
7	6.899	419	421	424	rBV	571048	495070	19.85%	3.265%
8	7.059	432	435	438	rBV	1984796	1766827	70.82%	11.653%
9	7.459	467	470	473	rBV	1094227	1337404	53.61%	8.821%
10	8.190	531	534	536	rBV	577869	615778	24.68%	4.061%
11	9.265	625	628	630	rBV	2707373	2494648	100.00%	16.454%
12	9.939	685	687	690	rBV	579930	583872	23.40%	3.851%
13	10.373	722	725	727	rBV	18293	28082	1.13%	0.185%
14	10.728	753	756	758	rBV	848786	838655	33.62%	5.531%
15	10.853	764	767	771	rVB	28478	38041	1.52%	0.251%
16	11.425	815	817	819	rBV	589461	543418	21.78%	3.584%
17	12.831	938	940	943	rBV	75279	71687	2.87%	0.473%
18	13.002	953	955	958	rBV	1675172	2203778	88.34%	14.535%
19	13.539	999	1002	1004	rBV	71050	63274	2.54%	0.417%
20	13.916	1032	1035	1041	rBV2	13494	27274	1.09%	0.180%
21	14.054	1045	1047	1054	rBV	500843	525778	21.08%	3.468%
22	15.494	1170	1173	1189	rBV	191769	373674	14.98%	2.465%

Sum of corrected areas: 15161666

LSC Report - Integrated Chromatogram

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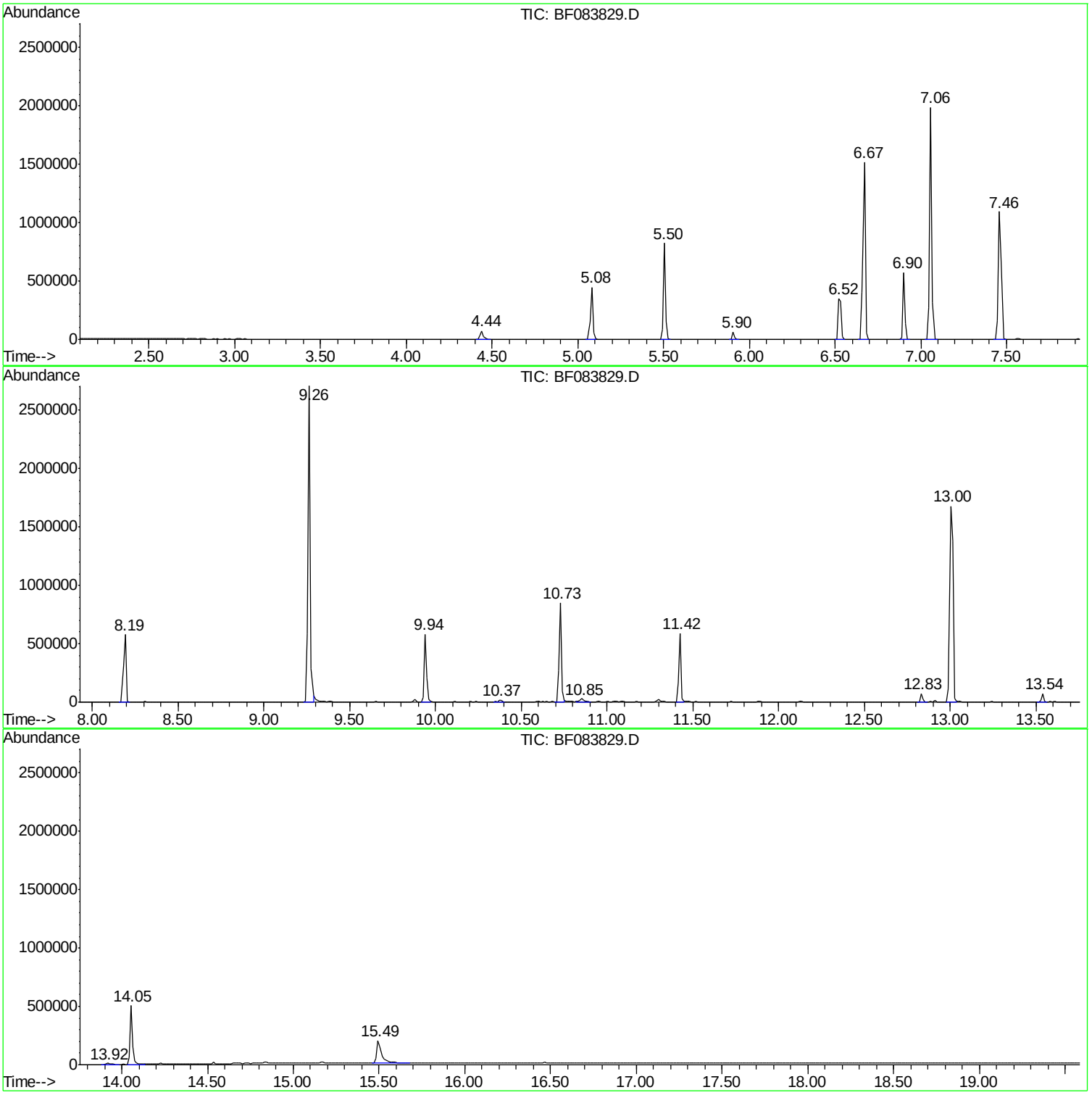
Operator : UM/IZ
Sample : G4782-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Data File : BF083829.D
Acq On : 15 Dec 2015 22:35
Operator : UM/IZ
Sample : G4782-01
Misc :
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Instrument : BNA_F
ClientSampleId : 121115-D534-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

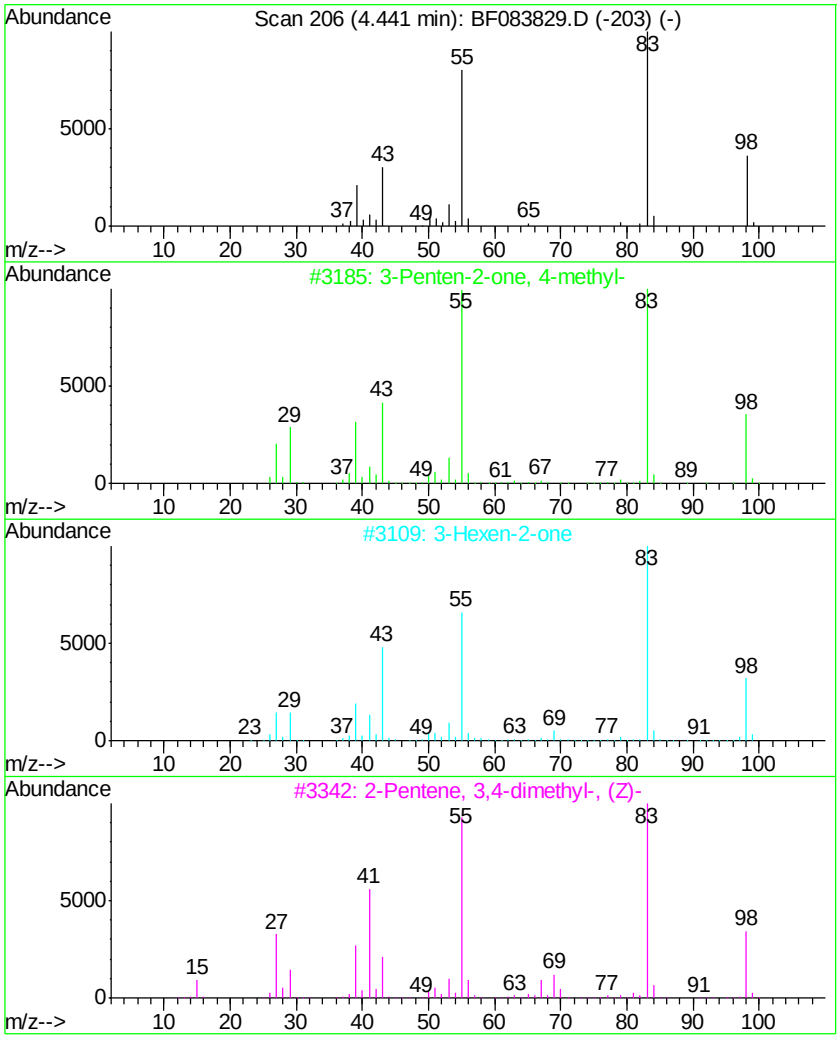
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

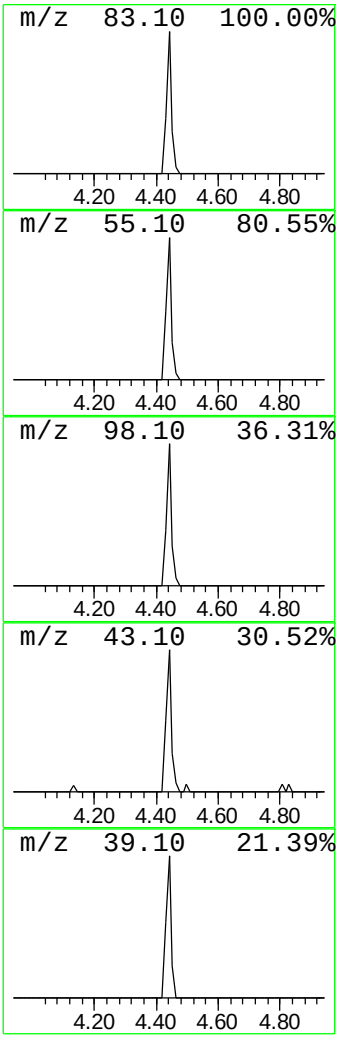
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	3.34 ng	82709	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80





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Data File : BF083829.D
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Operator : UM/IZ
Sample : G4782-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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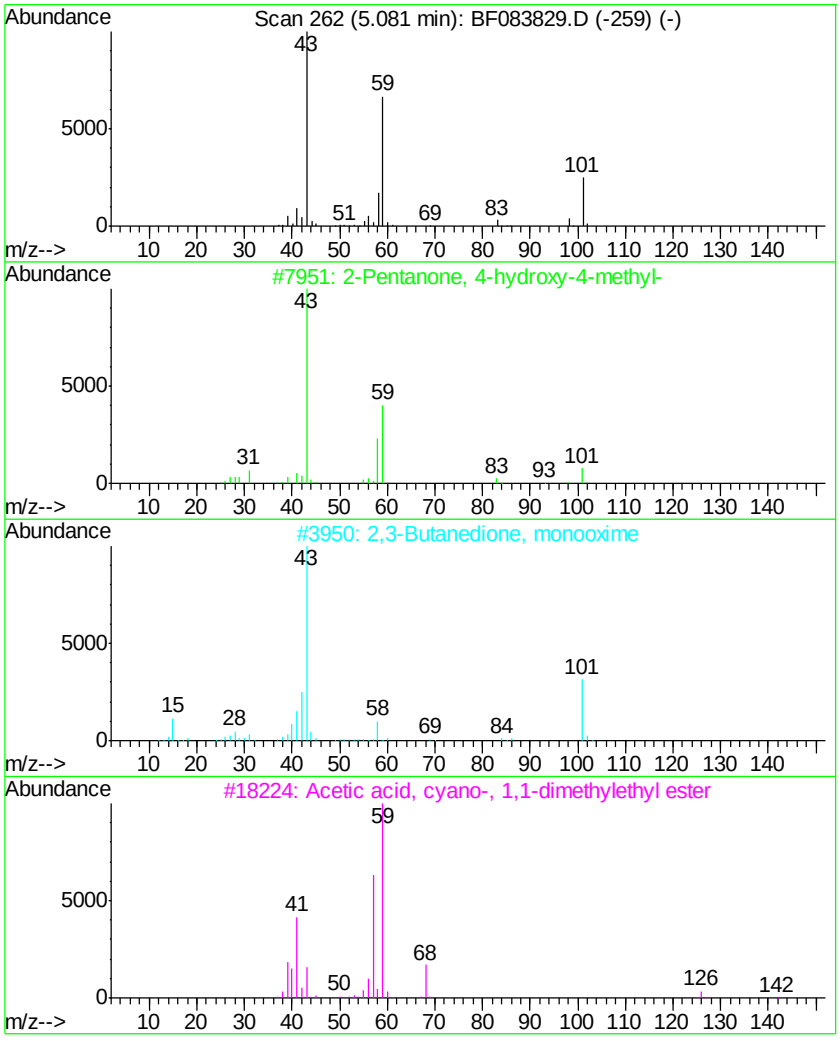
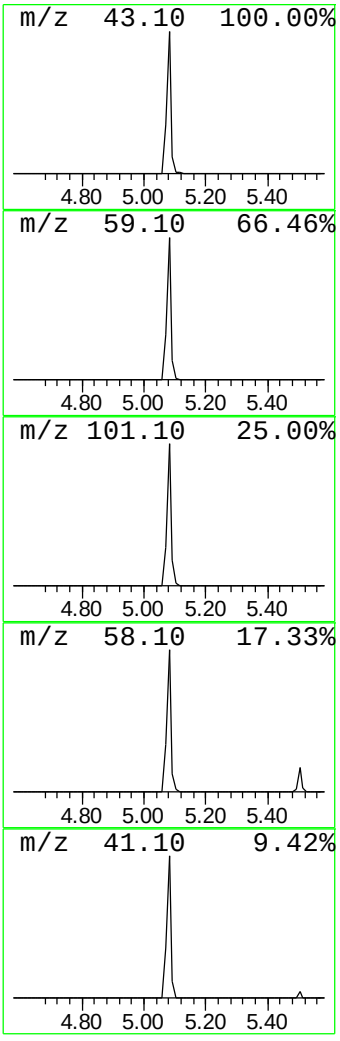
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	18.12 ng	448604	1,4-Dichlorobenzene-d4	6.90

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	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF083829.D
Acq On : 15 Dec 2015 22:35
Operator : UM/IZ
Sample : G4782-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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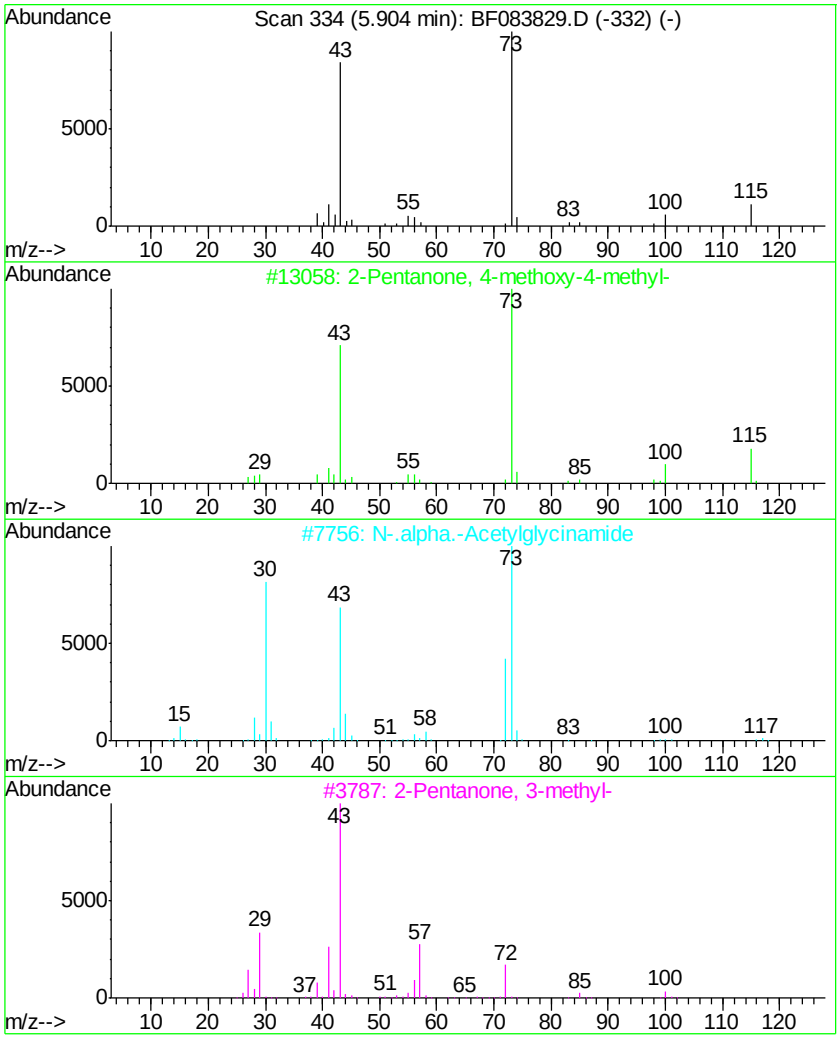
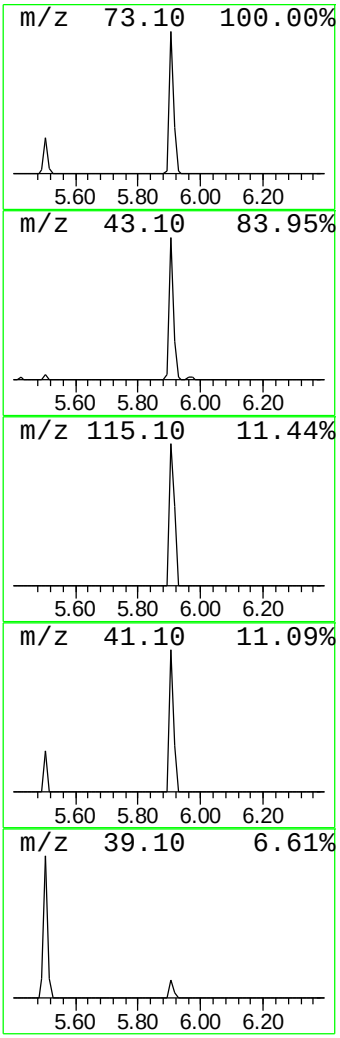
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.90	2.34 ng	57971	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4	Ethanone, 1-(3-ethyloxiranyl)-	114	C6H10O2	017257-81-7	10
5	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9





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Data File : BF083829.D
Acq On : 15 Dec 2015 22:35
Operator : UM/IZ
Sample : G4782-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
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TIC Library : C:\DATABASE\NIST02.L
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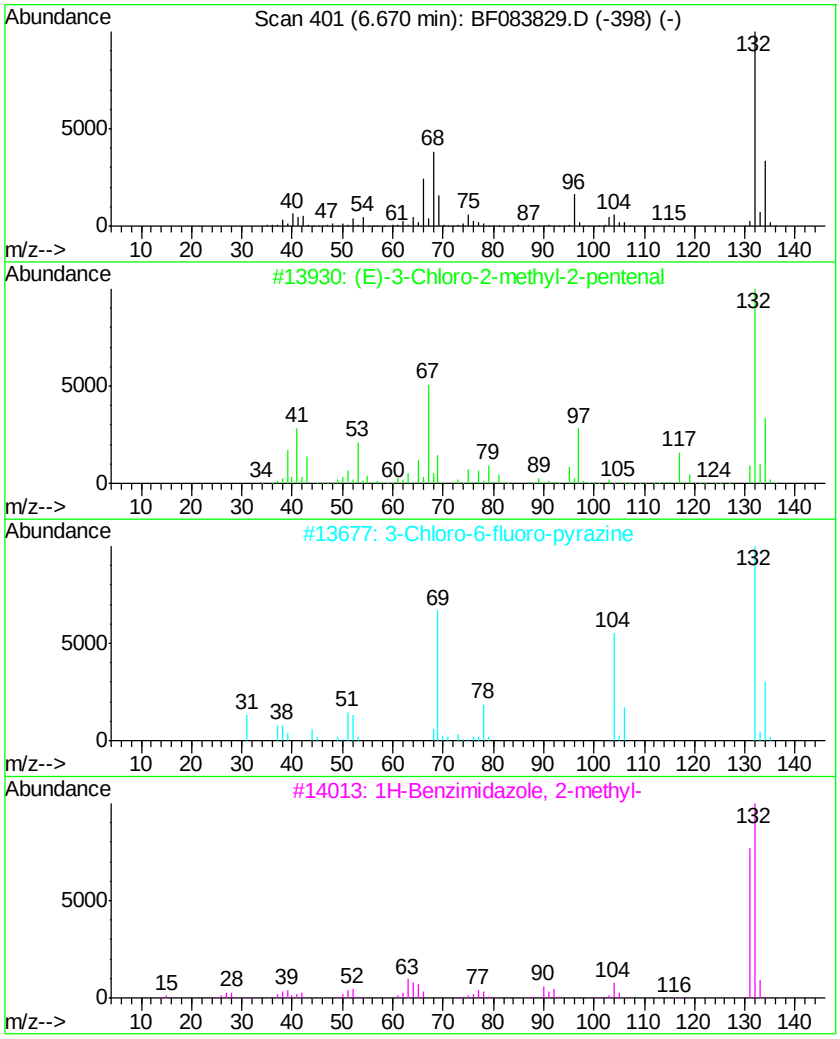
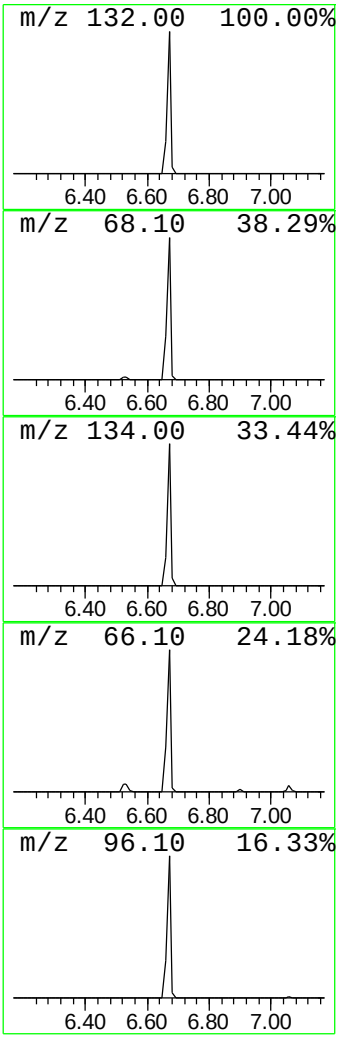
Peak Number 4 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	54.80 ng	1356580	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : G4782-01
Misc :
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Instrument : BNA_F
ClientSampleId : 121115-D534-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

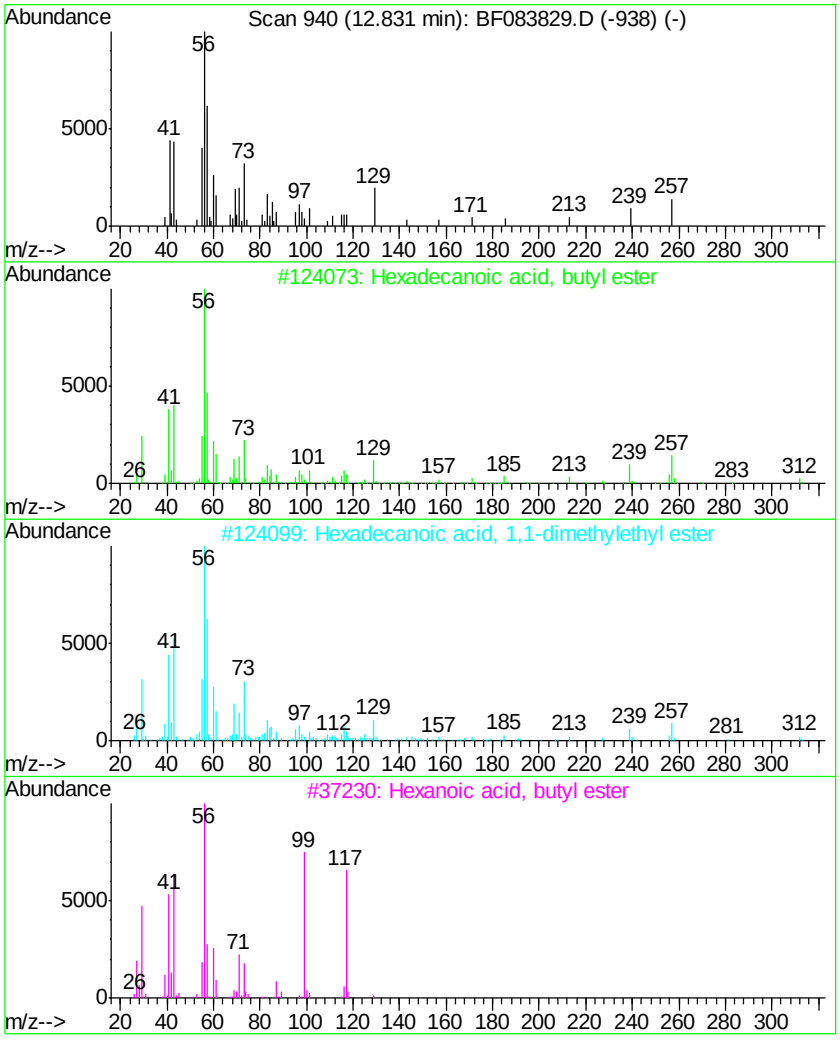
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

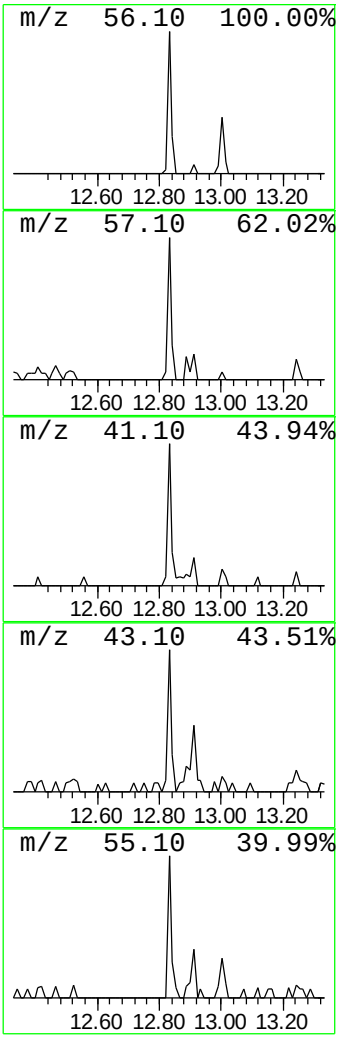
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	2.73 ng	71687	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Hexanoic acid, butyl ester	172	C10H20O2	000626-82-4	40
4	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
5	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35





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Operator : UM/IZ
Sample : G4782-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

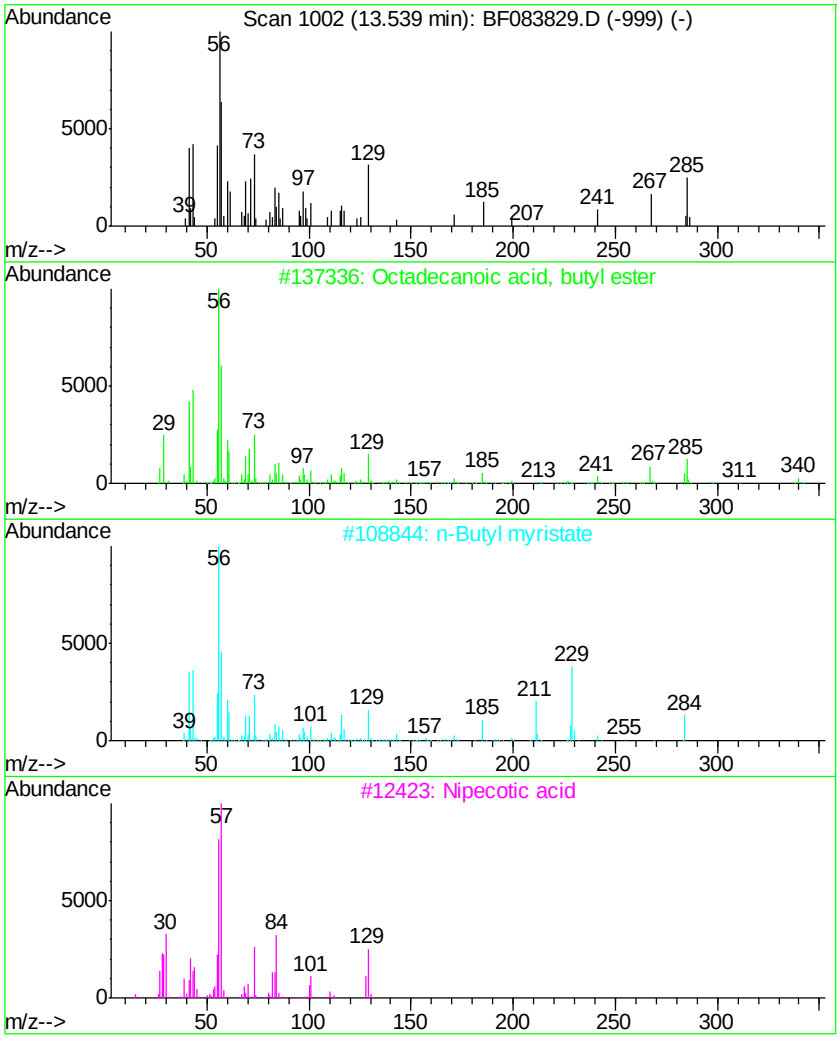
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

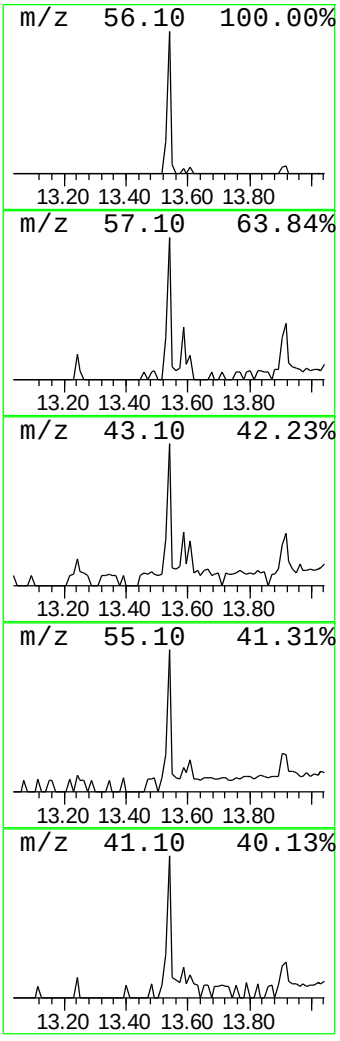
****

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	2.41 ng	63274	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	80
2	n-Butyl myristate	284	C18H36O2	000110-36-1	53
3	Nipecotic acid	129	C6H11NO2	000498-95-3	38
4	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	32
5	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	32





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.44	3.3	ng	82709	1	6.90	495070	20.0
2-Pentanone, 4-hy...	5.08	18.1	ng	448604	1	6.90	495070	20.0
2-Pentanone, 4-me...	5.90	2.3	ng	57971	1	6.90	495070	20.0
unknown6.67	6.67	54.8	ng	1356580	1	6.90	495070	20.0
Hexadecanoic acid...	12.83	2.7	ng	71687	5	14.05	525778	20.0
Octadecanoic acid...	13.54	2.4	ng	63274	5	14.05	525778	20.0