LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083834.D
Acq On : 16 Dec 2015 00:55
Operator : UM/IZ
Sample : G4782-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-U-S

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	211	rVB	50823	77743	2.91%	0.496%
2	5.081	259	262	264	rBV	307671	383759	14.39%	2.447%
3	5.504	297	299	301	rBV	752957	680899	25.52%	4.341%
4	5.904	332	334	337	rBB	66162	54404	2.04%	0.347%
5	6.521	386	388	391	rBV	406857	398945	14.95%	2.543%
6	6.670	398	401	403	rBV	1389700	1320299	49.49%	8.417%
7	6.899	419	421	424	rBB	628200	531885	19.94%	3.391%
8	7.059	433	435	437	rBV	2016143	1741882	65.30%	11.105%
9	7.459	467	470	473	rBV	1132028	1304957	48.92%	8.319%
10	8.190	531	534	536	rBV	592256	663415	24.87%	4.229%
11	9.265	625	628	630	rBV	2915618	2667671	100.00%	17.007%
12	9.939	685	687	690	rBV	729337	685188	25.68%	4.368%
13	10.728	753	756	758	rBV	964787	949128	35.58%	6.051%
14	10.853	765	767	771	rVB	30070	40694	1.53%	0.259%
15	11.425	815	817	819	rBV	697116	637786	23.91%	4.066%
16	12.831	938	940	942	rBV	77377	67340	2.52%	0.429%
17	12.911	942	947	949	rVB2	29391	33338	1.25%	0.213%
18	13.002	953	955	958	rBV	1810506	2334571	87.51%	14.883%
19	13.539	1000	1002	1004	rBV	62330	54049	2.03%	0.345%
20	13.905	1032	1034	1040	rBV	29125	58056	2.18%	0.370%
21	14.054	1044	1047	1055	rVV	544304	566856	21.25%	3.614%
22	15.494	1170	1173	1188	rBV	214526	400544	15.01%	2.554%
23	16.465	1254	1258	1264	rBV6	10747	32270	1.21%	0.206%

Sum of corrected areas: 15685679

LSC Report - Integrated Chromatogram

Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
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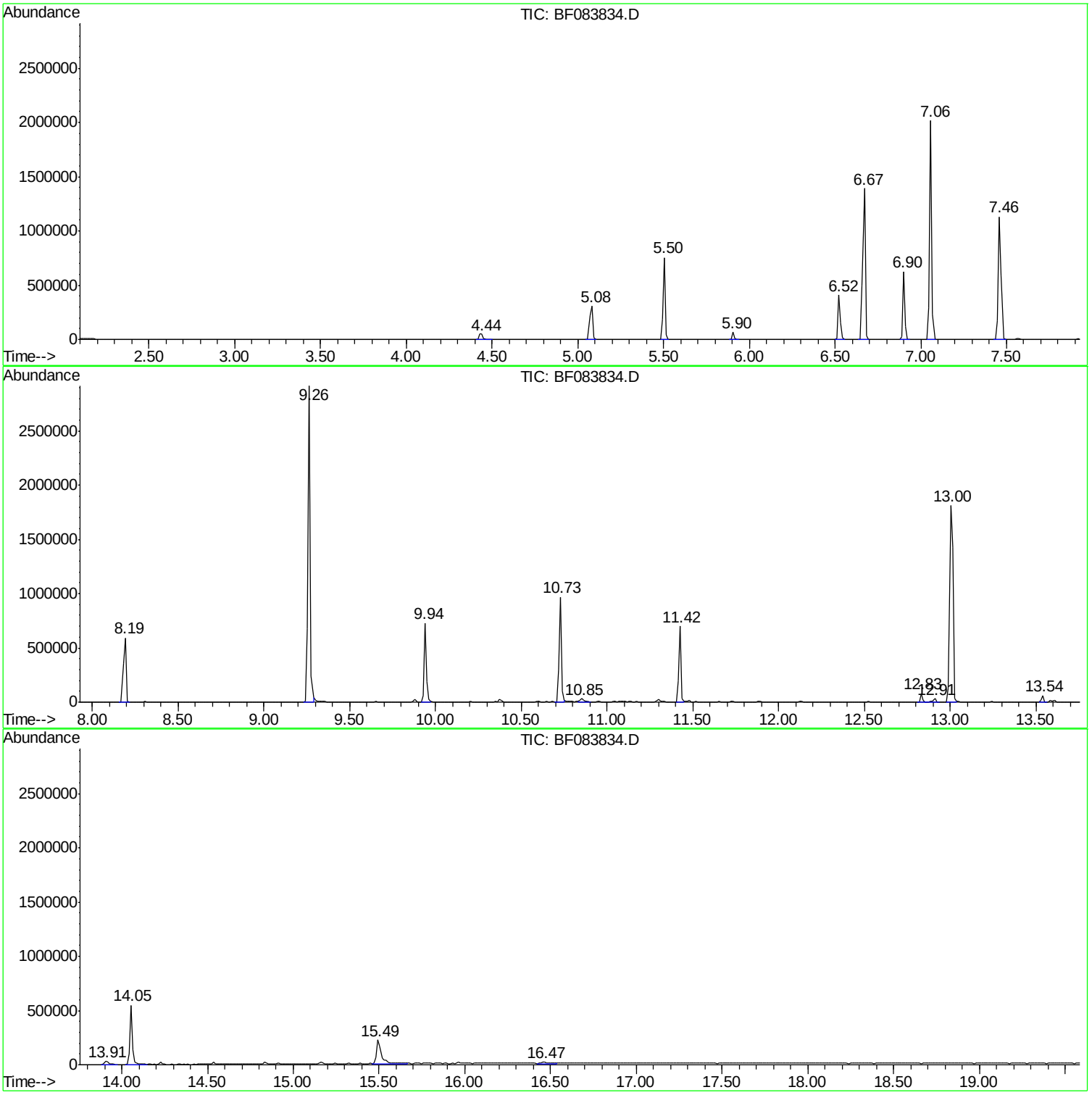
Operator : UM/IZ
Sample : G4782-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-U-S

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



Library Search Compound Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083834.D
Acq On : 16 Dec 2015 00:55
Operator : UM/IZ
Sample : G4782-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-U-S

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

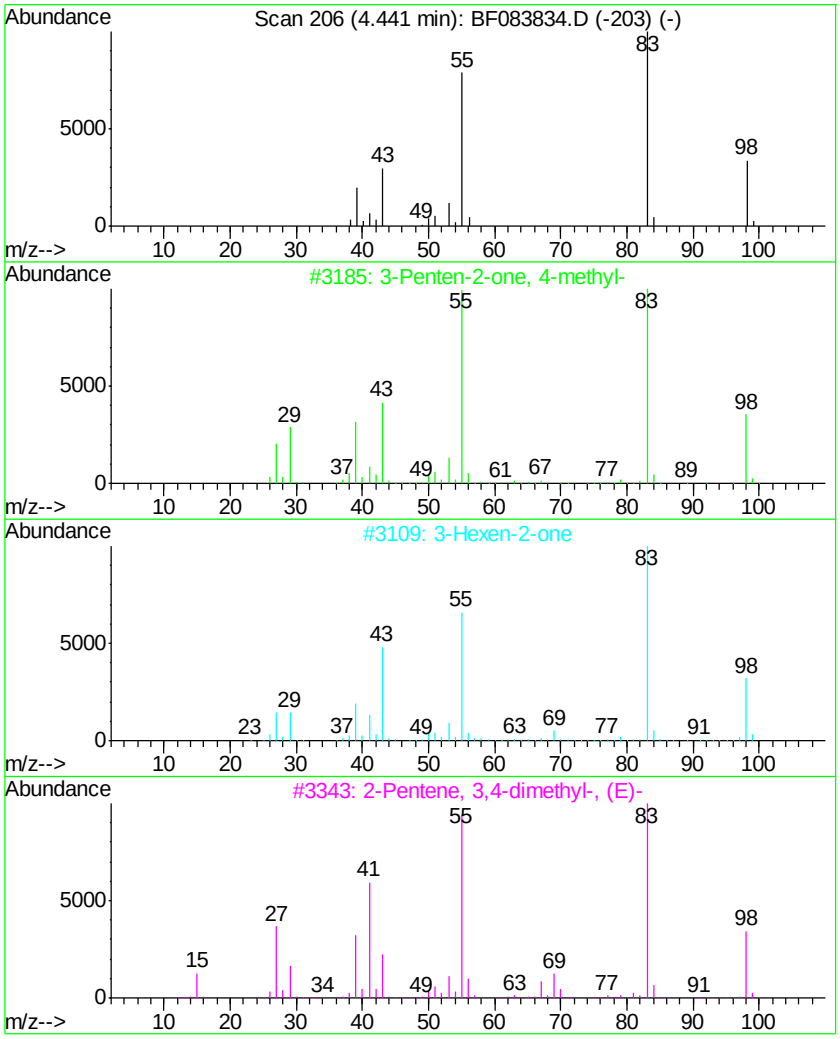
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

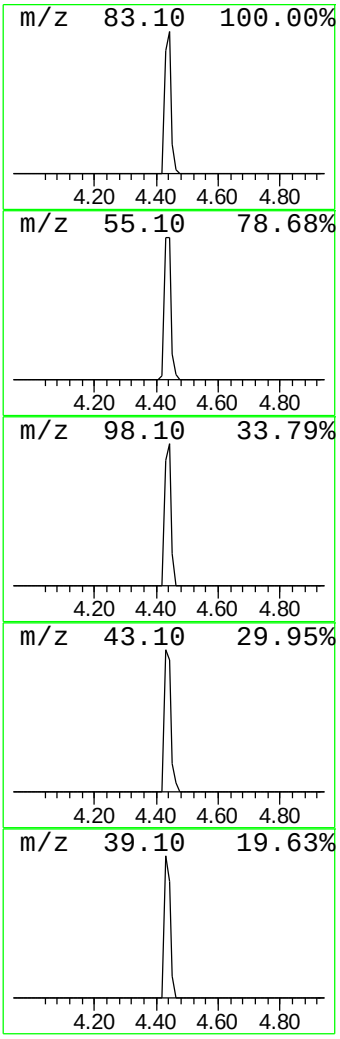
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	2.92 ng	77743	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-, (E)-	98	C7H14	004914-92-5	78
4	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72





Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083834.D
Acq On : 16 Dec 2015 00:55
Operator : UM/IZ
Sample : G4782-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-U-S

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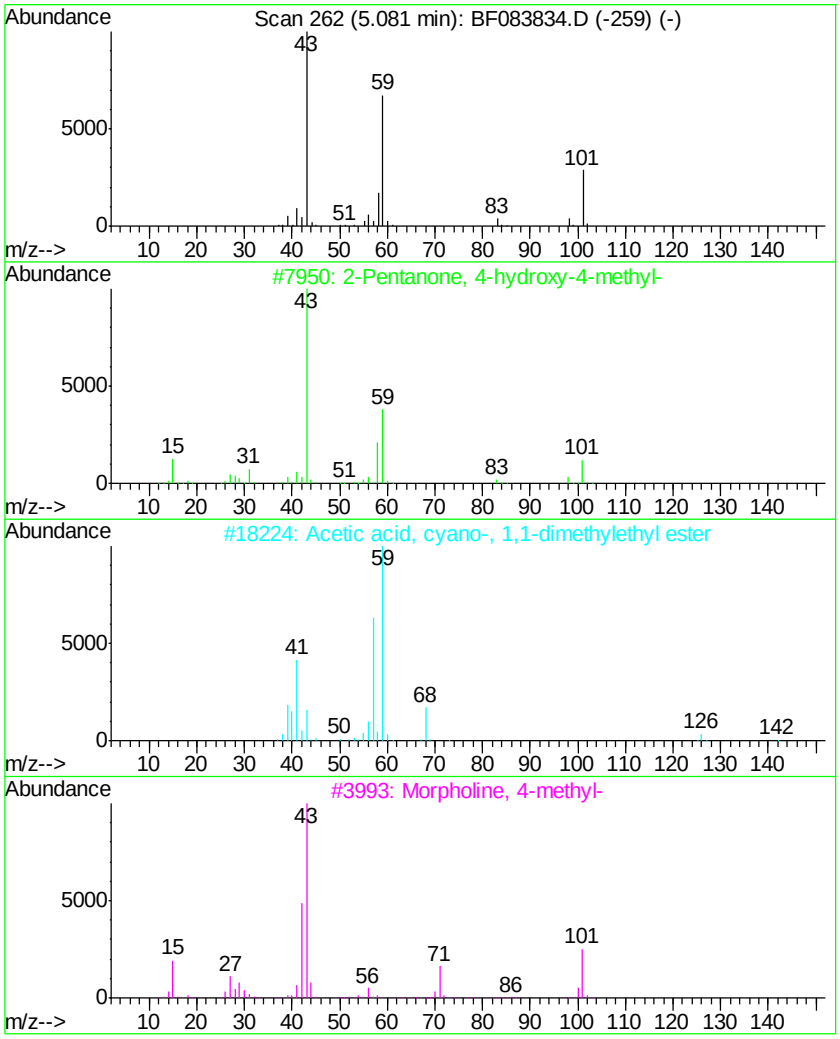
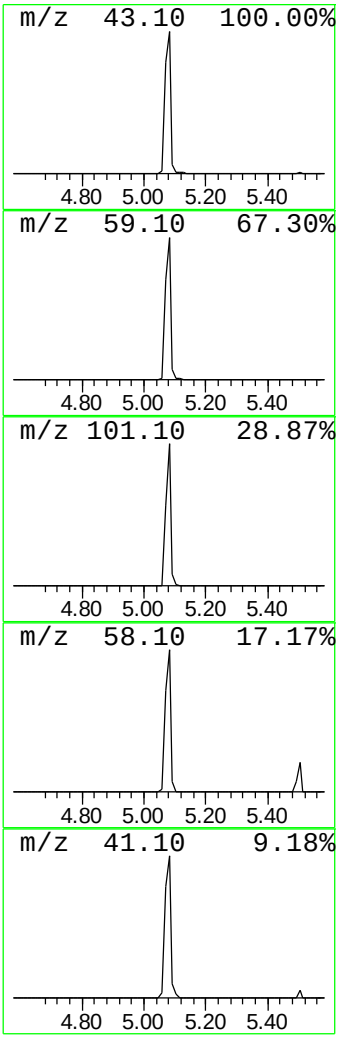
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	14.43 ng	383759	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083834.D
Acq On : 16 Dec 2015 00:55
Operator : UM/IZ
Sample : G4782-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-U-S

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

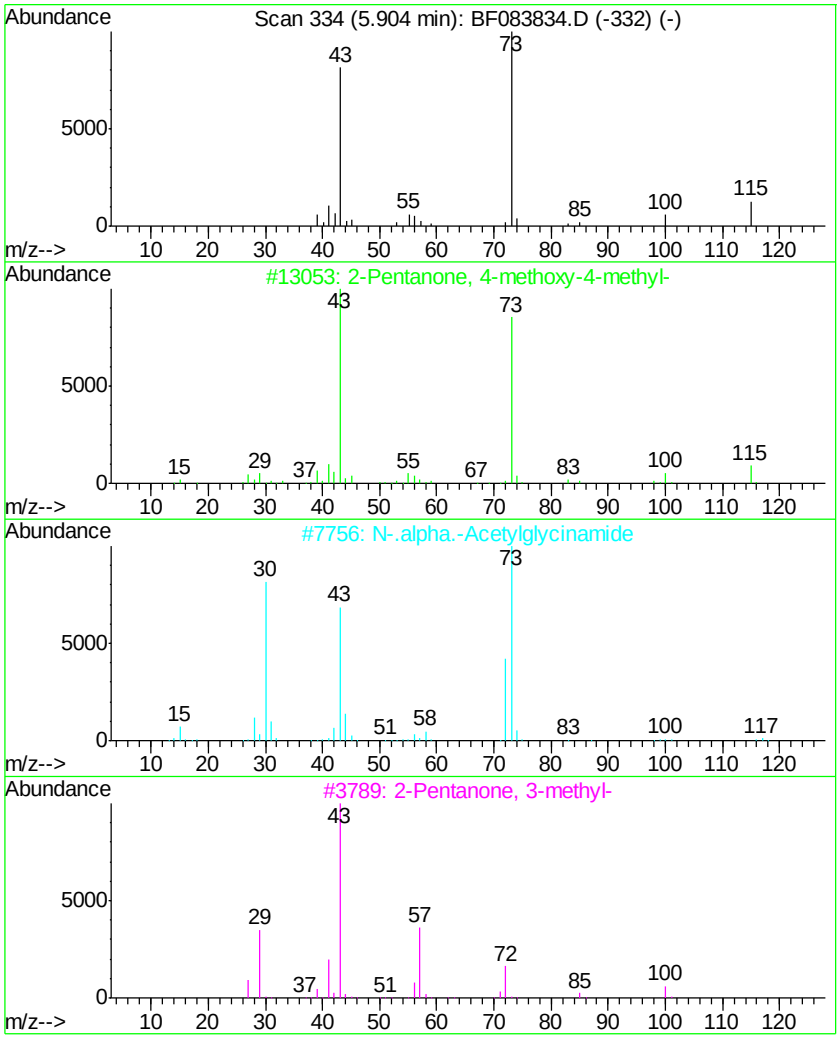
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

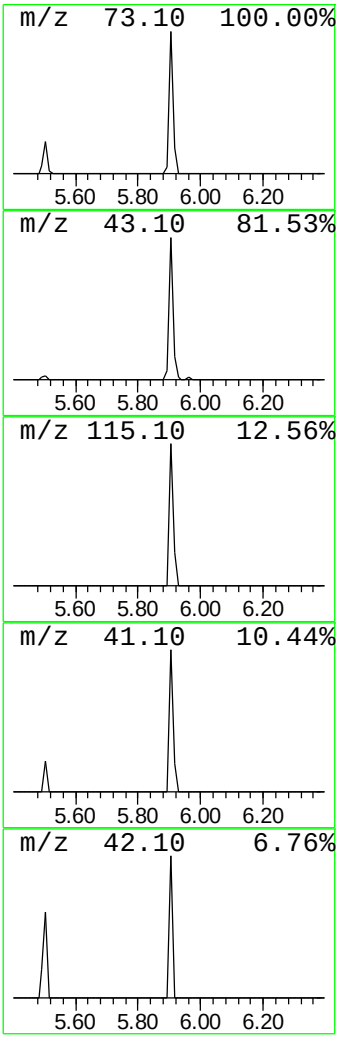
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.90	2.05 ng	54404	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	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	Hexane, 2-methyl-	100	C7H16	000591-76-4	9





Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083834.D
Acq On : 16 Dec 2015 00:55
Operator : UM/IZ
Sample : G4782-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-U-S

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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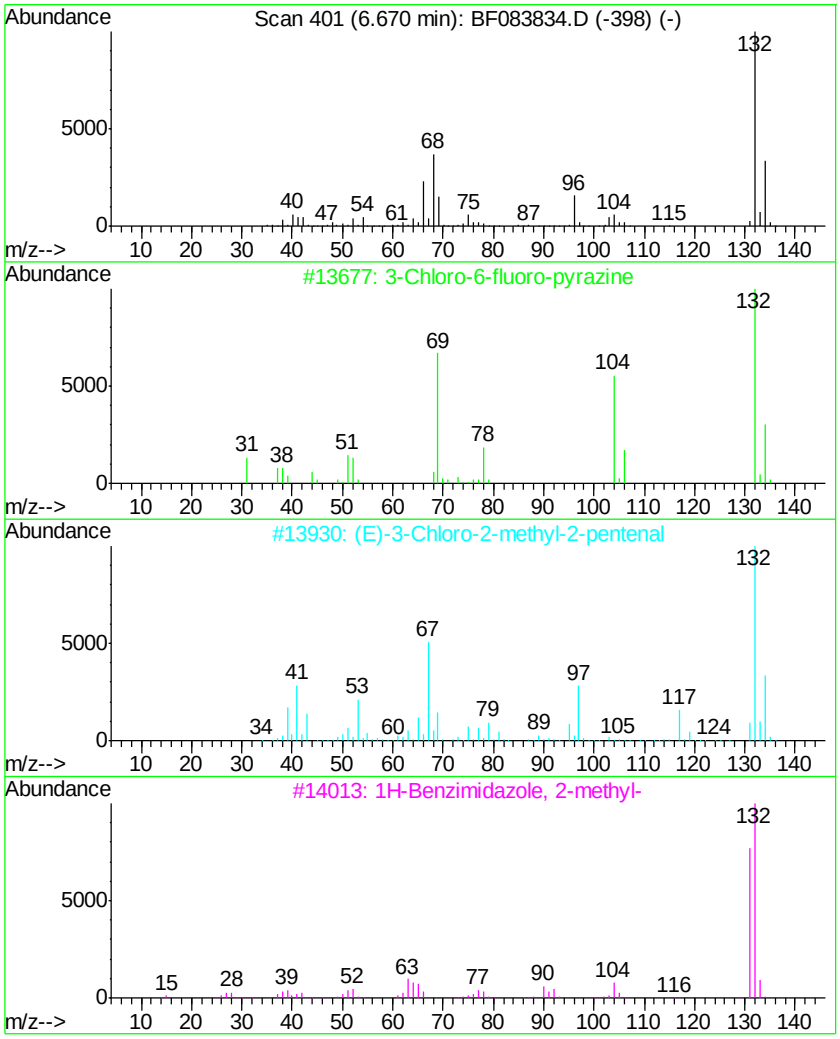
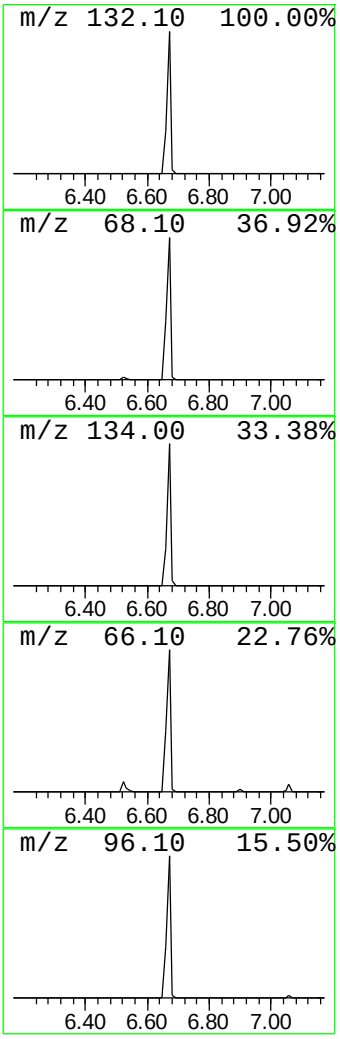
Peak Number 4 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	49.65 ng	1320300	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : V:\HPCHEM1\BNA F\DATA\BF121515\
Data File : BF083834.D
Acq On : 16 Dec 2015 00:55
Operator : UM/IZ
Sample : G4782-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-U-S

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

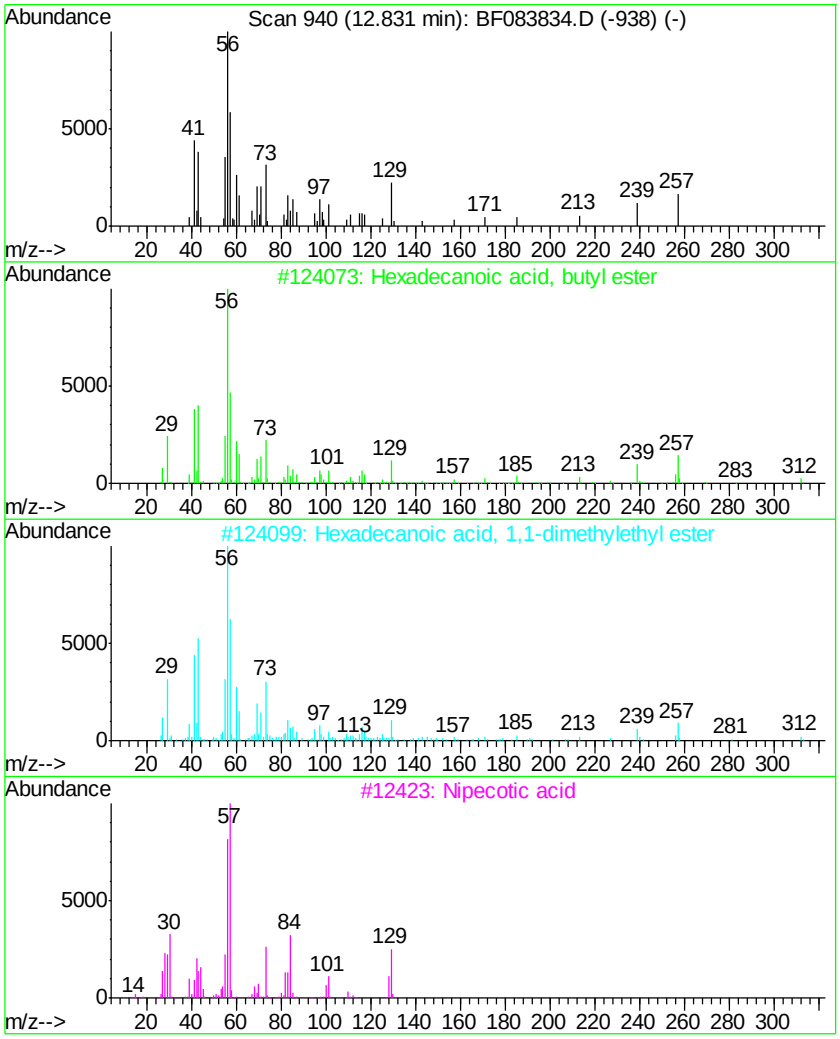
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

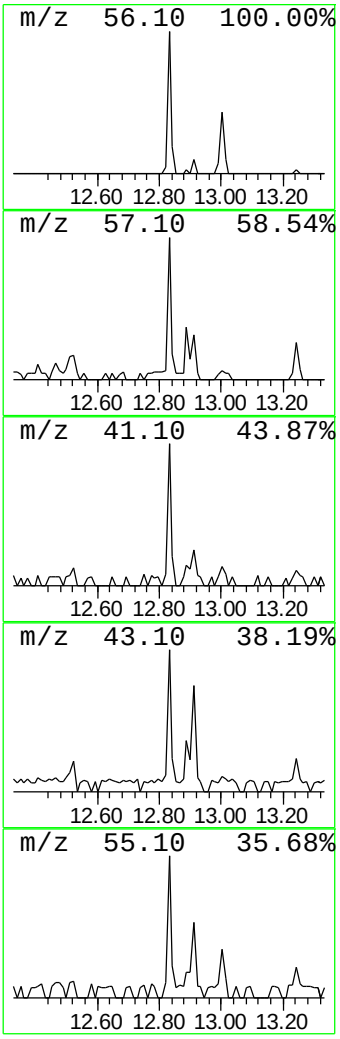
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	2.38 ng	67340	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	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Hexanoic acid, butyl ester	172	C10H20O2	000626-82-4	38
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32





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Sample : G4782-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121115-D534-F-U-S

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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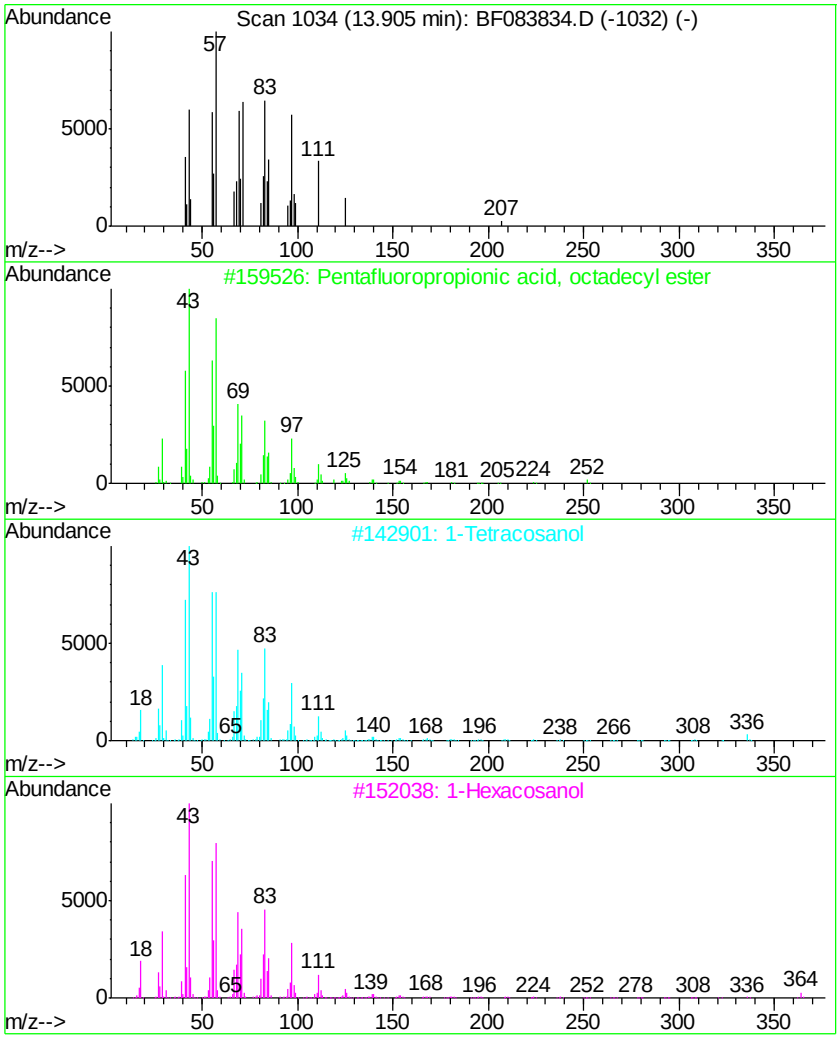
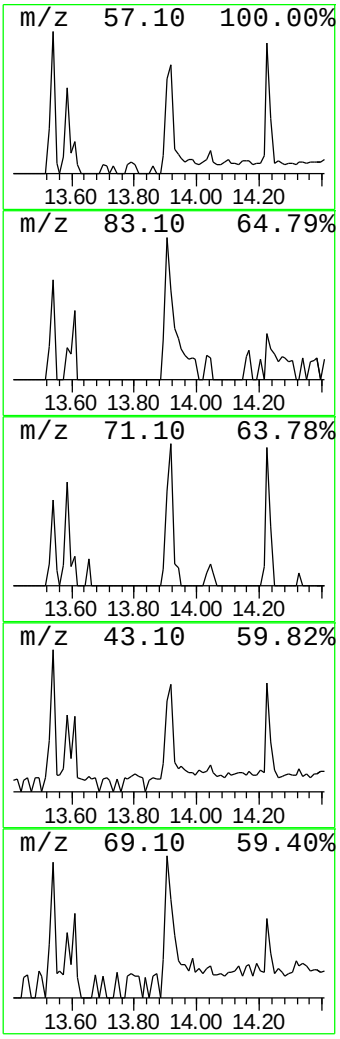
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	2.05 ng	58056	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	90
2	1-Tetracosanol	354	C24H50O	000506-51-4	74
3	1-Hexacosanol	382	C26H54O	000506-52-5	62
4	1-Nonadecene	266	C19H38	018435-45-5	59
5	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	59





Tentatively Identified Compound (LSC) summary

Data Path : V:\HPCHEM1\BNA_F\DATA\BF121515\
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.44	2.9	ng	77743	1	6.90	531885	20.0
2-Pentanone, 4-hy...	5.08	14.4	ng	383759	1	6.90	531885	20.0
2-Pentanone, 4-me...	5.90	2.0	ng	54404	1	6.90	531885	20.0
unknown6.67	6.67	49.6	ng	1320300	1	6.90	531885	20.0
Hexadecanoic acid...	12.83	2.4	ng	67340	5	14.05	566856	20.0
Pentafluoropropio...	13.91	2.0	ng	58056	5	14.05	566856	20.0