LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092315.D
Acq On : 17 Jan 2017 7:29
Operator : UM/SJ
Sample : I1219-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

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-BF122116.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	2.210	35	37	48	rVB	219888	358734	5.29%	0.674%
2	2.850	90	93	100	rBV	149255	279147	4.11%	0.525%
3	3.958	187	190	205	rBV	1840607	3010767	44.38%	5.659%
4	4.701	253	255	270	rBV	1017914	2004300	29.54%	3.767%
5	4.987	278	280	288	rVB	92451	130400	1.92%	0.245%
6	5.170	294	296	307	rBV	4675290	5649730	83.27%	10.619%
7	6.233	386	389	396	rBV	4254125	4586523	67.60%	8.620%
8	6.336	396	398	401	rVV	4467100	5137091	75.72%	9.655%
9	6.564	416	418	421	rBV	1101308	995898	14.68%	1.872%
10	6.724	429	432	434	rBV	3458947	4403196	64.90%	8.276%
11	7.136	466	468	471	rBV	3176818	3290119	48.49%	6.184%
12	7.845	528	530	533	rBV	1162964	1374045	20.25%	2.582%
13	8.930	622	625	627	rBV	6928165	6784459	100.00%	12.751%
14	9.593	681	683	685	rBV	1970169	1750145	25.80%	3.289%
15	10.382	749	752	755	rBV	3128033	3755311	55.35%	7.058%
16	11.068	810	812	815	rBV	1638140	1569367	23.13%	2.950%
17	12.496	934	937	939	rBV	138452	121725	1.79%	0.229%
18	12.656	948	951	954	rBV	5046550	4848542	71.47%	9.113%
19	13.697	1039	1042	1045	rBV	1225049	1156378	17.04%	2.173%
20	15.045	1158	1160	1163	rBV	786236	1183670	17.45%	2.225%
21	15.091	1163	1164	1170	rVB	97109	98990	1.46%	0.186%
22	15.445	1193	1195	1198	rBV	95370	131908	1.94%	0.248%
23	15.857	1228	1231	1237	rVB	107715	182084	2.68%	0.342%
24	16.337	1269	1273	1277	rBV	78468	155514	2.29%	0.292%
25	16.897	1318	1322	1328	rVB	63009	151202	2.23%	0.284%
26	17.560	1376	1380	1385	rBV	35214	96783	1.43%	0.182%

Sum of corrected areas: 53206028

LSC Report - Integrated Chromatogram

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Data File : BF092315.D
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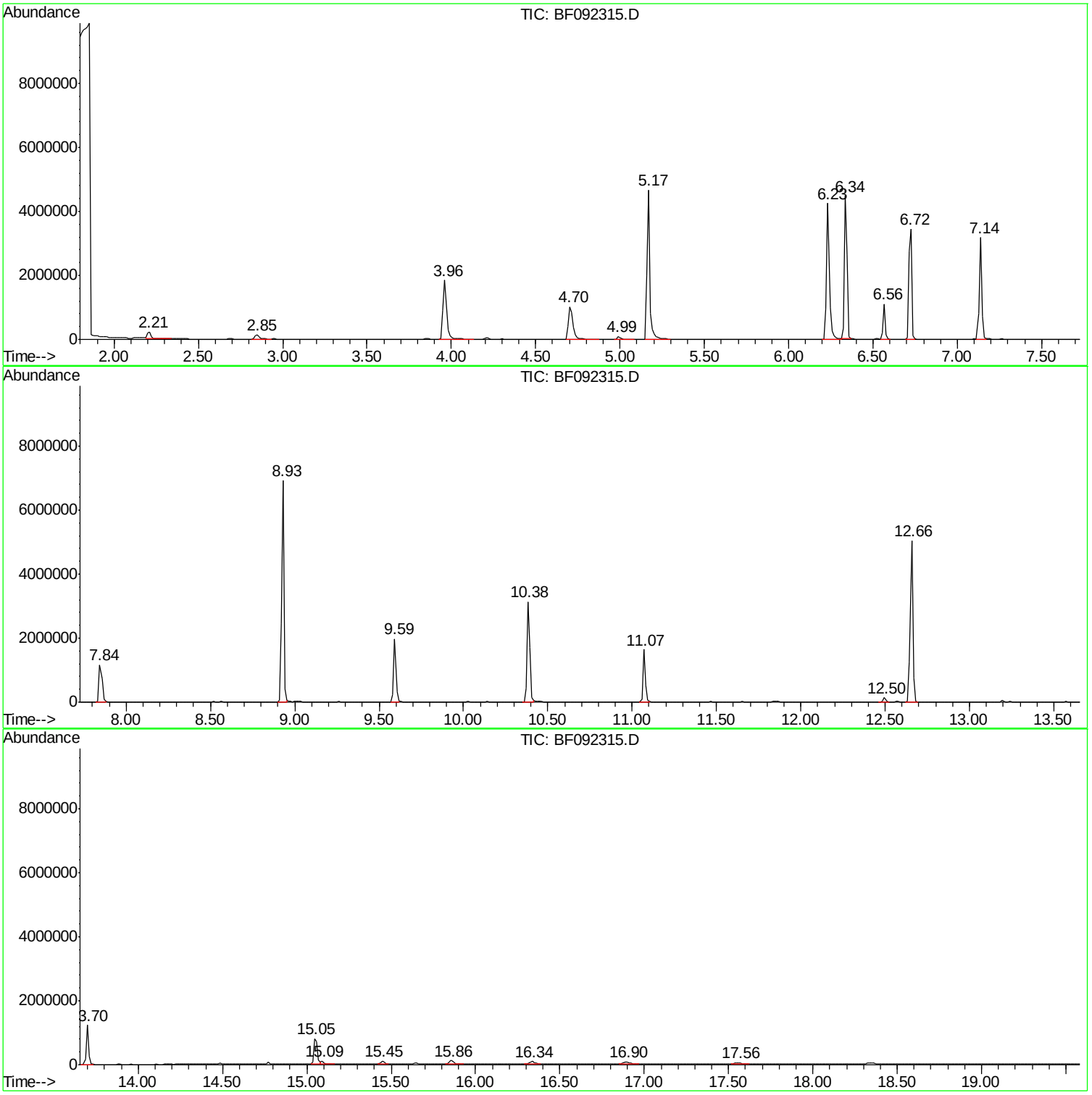
Operator : UM/SJ
Sample : I1219-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092315.D
Acq On : 17 Jan 2017 7:29
Operator : UM/SJ
Sample : I1219-01
Misc :
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Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

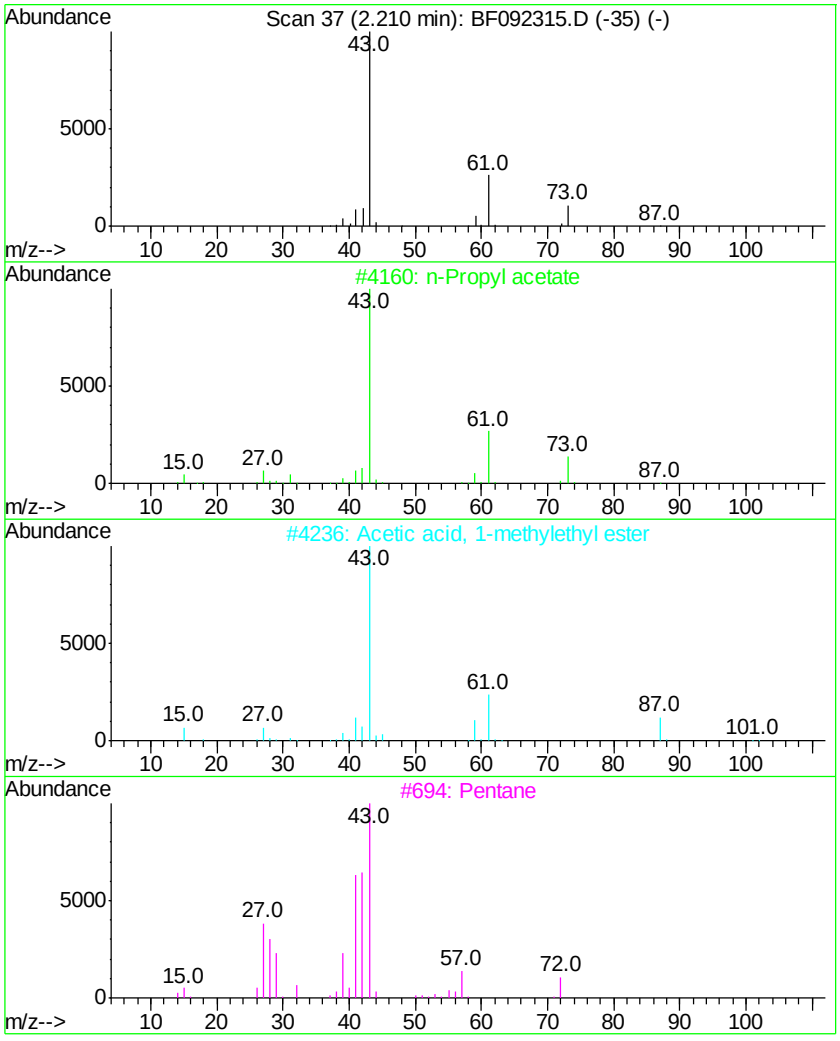
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

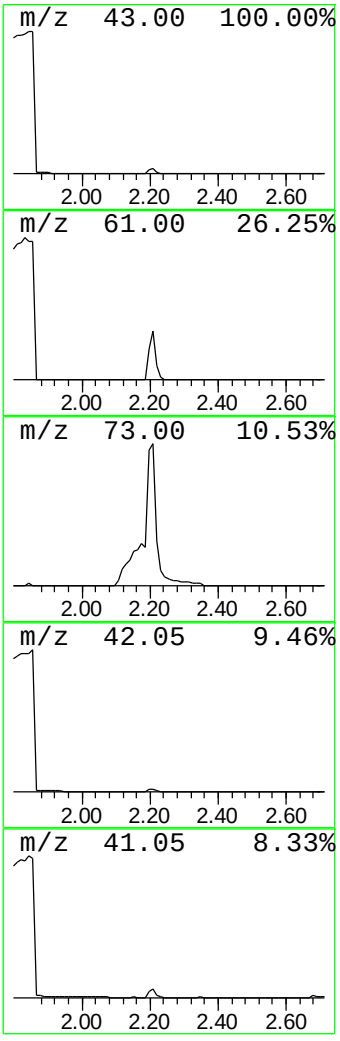
****

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	7.20 ng	358734	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	9
3	Pentane	72	C5H12	000109-66-0	5
4	Isobutylamine	73	C4H11N	000078-81-9	4
5	1-Butanamine	73	C4H11N	000109-73-9	4





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Acq On : 17 Jan 2017 7:29
Operator : UM/SJ
Sample : I1219-01
Misc :
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Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

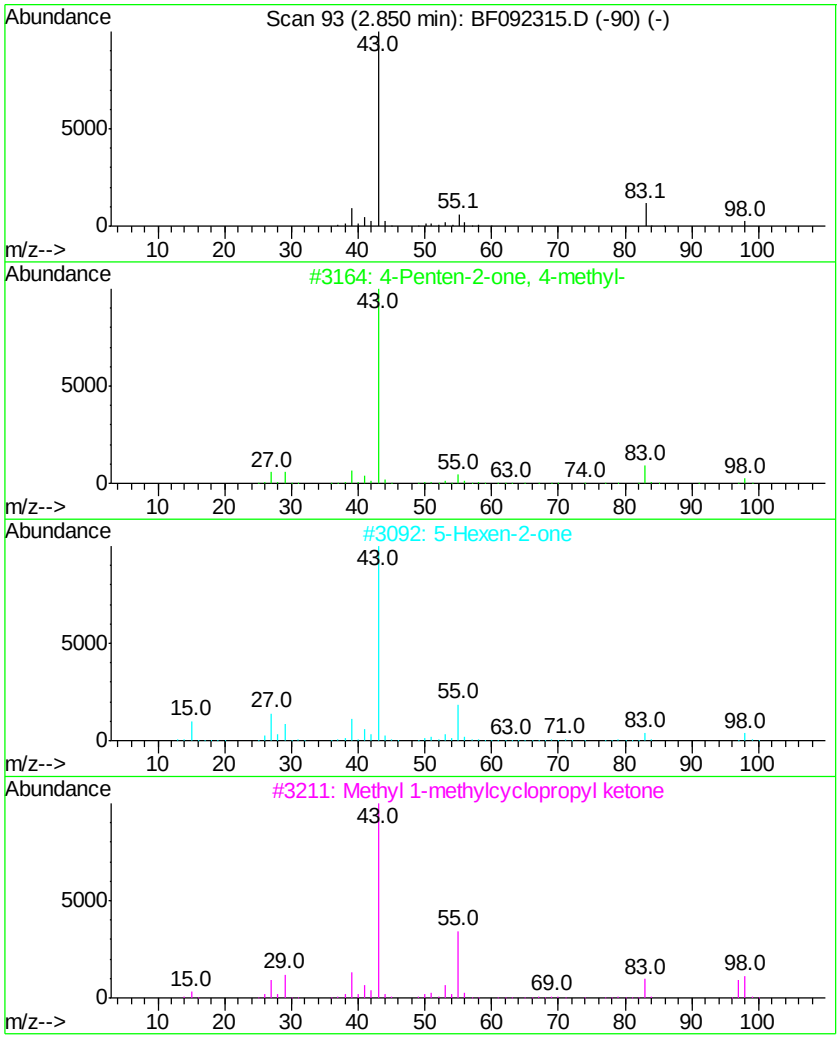
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

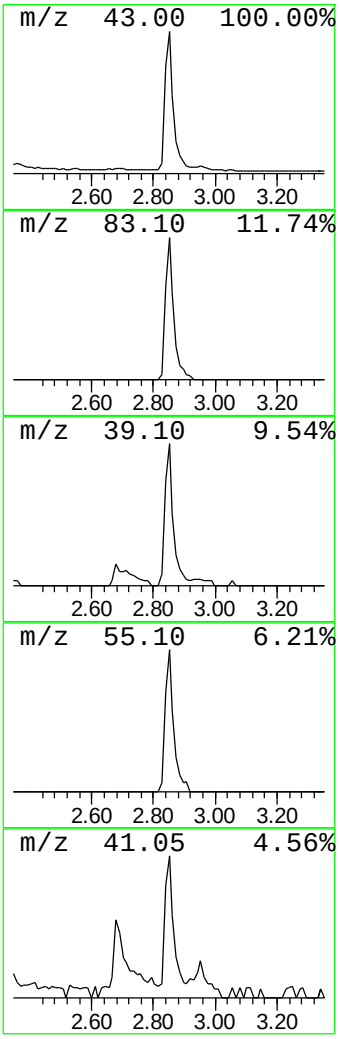
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	5.61 ng	279147	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	38
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	35
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	28
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092315.D
Acq On : 17 Jan 2017 7:29
Operator : UM/SJ
Sample : I1219-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

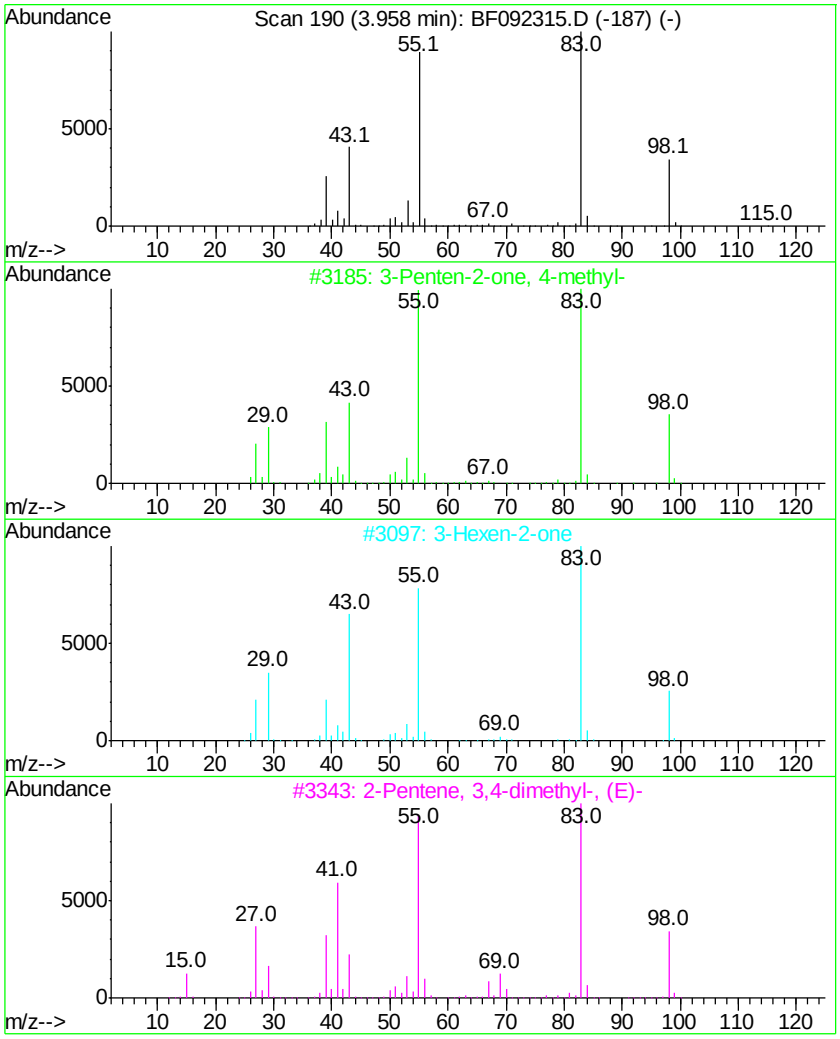
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

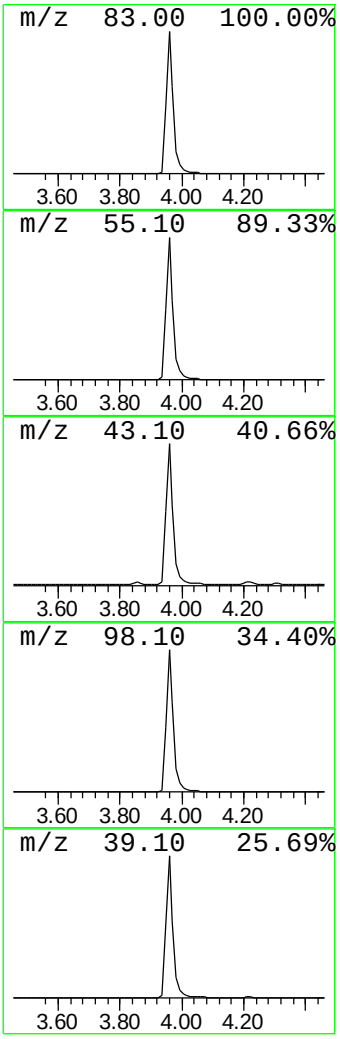
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.96	60.46 ng	3010770	1,4-Dichlorobenzene-d4	6.56

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	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Operator : UM/SJ
Sample : I1219-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

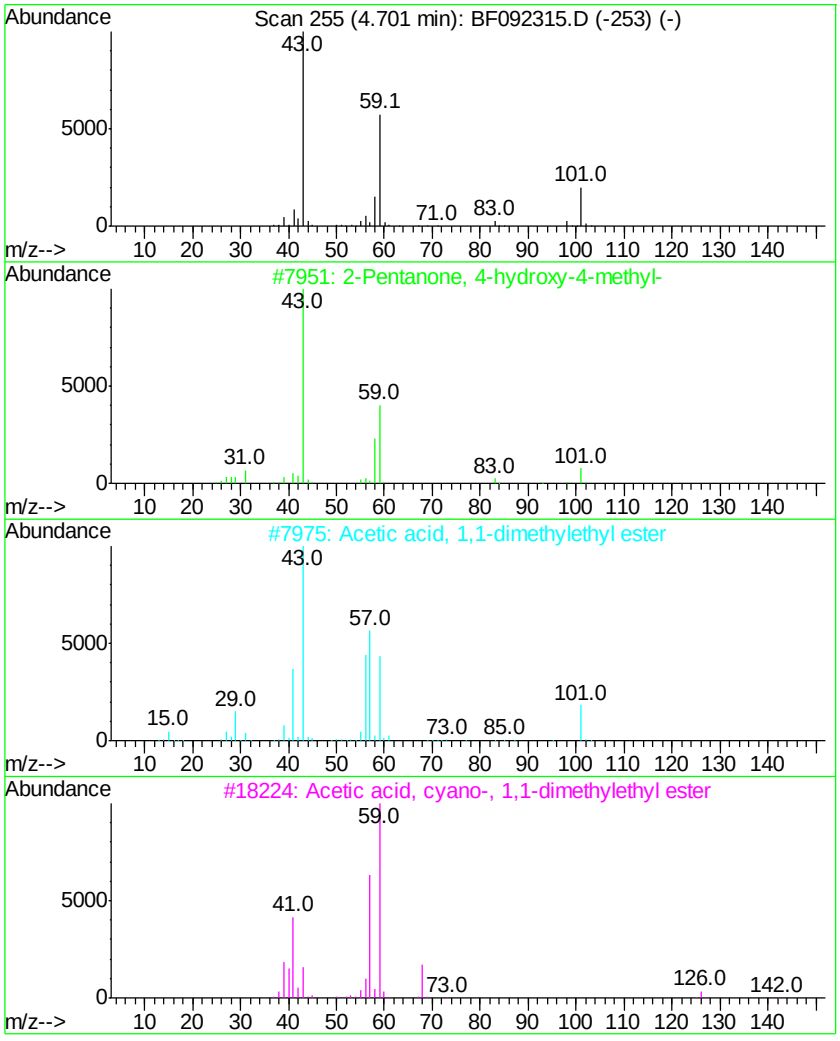
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

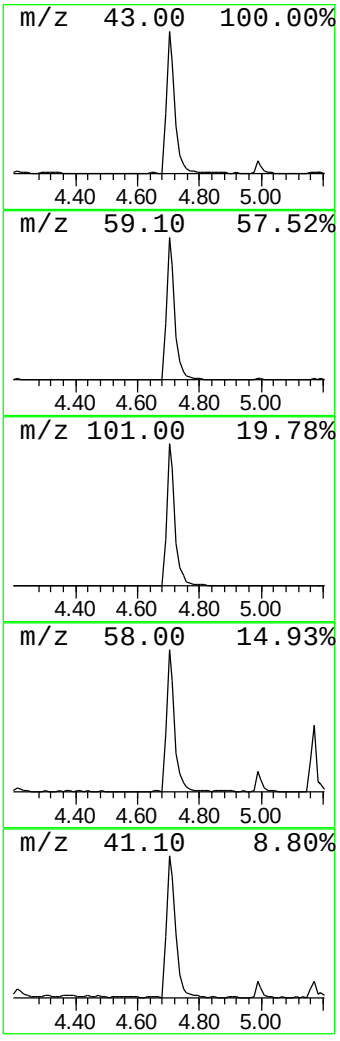
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	40.25 ng	2004300	1,4-Dichlorobenzene-d4	6.56

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
Data File : BF092315.D
Acq On : 17 Jan 2017 7:29
Operator : UM/SJ
Sample : I1219-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

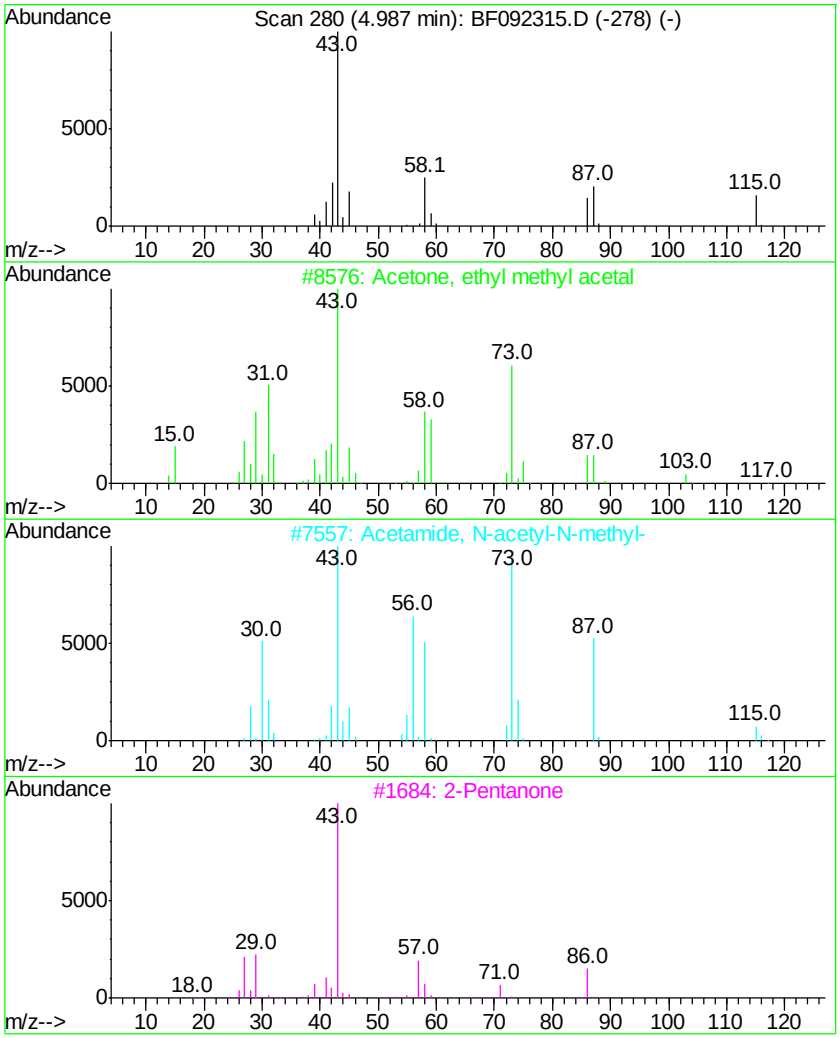
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

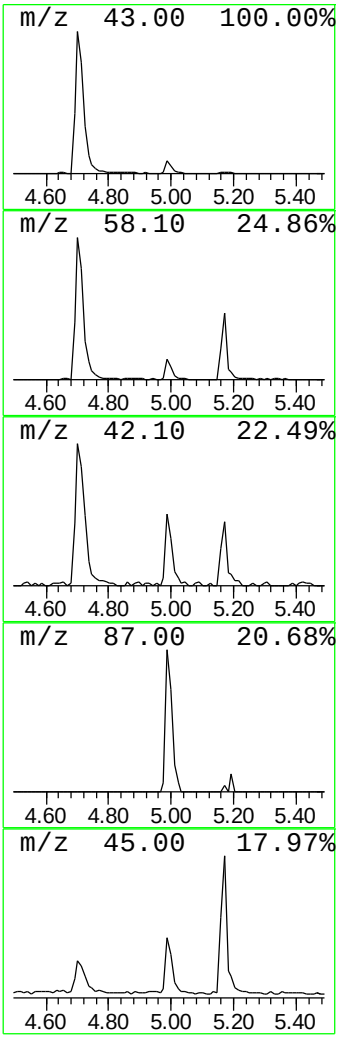
****

Peak Number 5 unknown4.99 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	2.62 ng	130400	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetone, ethyl methyl acetal	118	C6H14O2	029328-22-1	33
2	Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9
3	2-Pentanone	86	C5H10O	000107-87-9	9
4	Oxirane-2-carboxylic acid, ethyl...	116	C5H8O3	1000192-50-3	9
5	1,3-Dioxolane, 2,2,4,5-tetrameth...	130	C7H14O2	017226-66-3	9





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Sample : I1219-01
Misc :
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Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

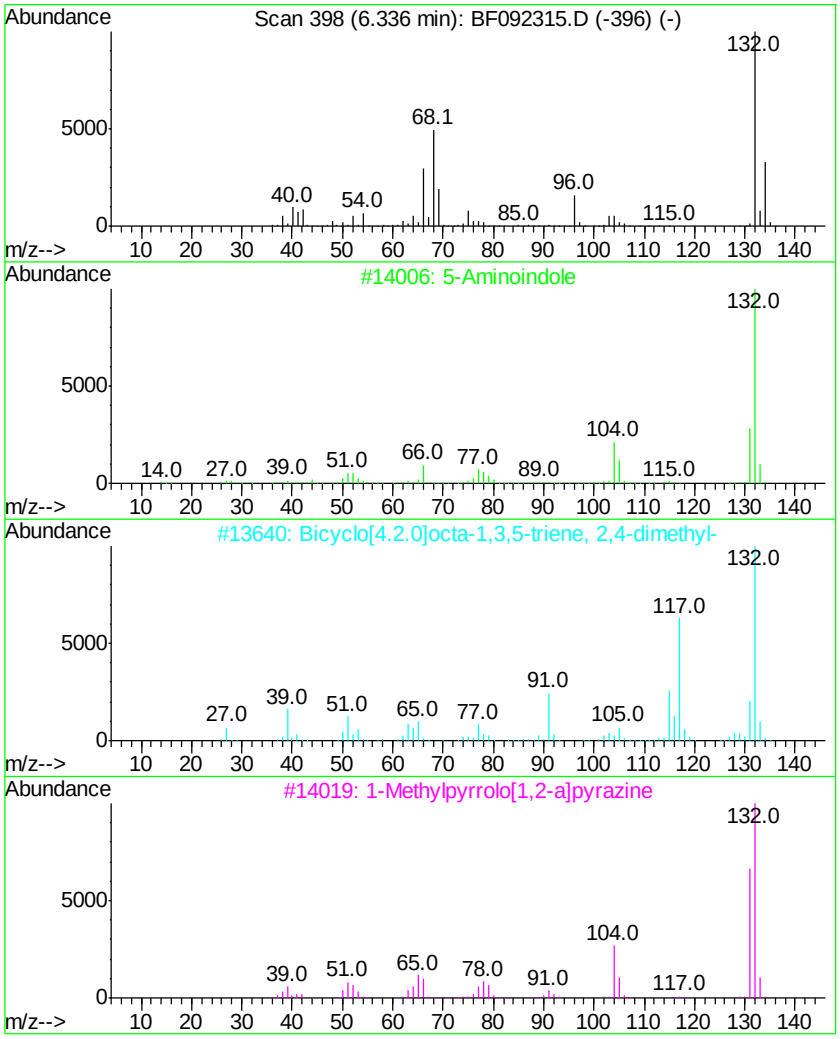
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

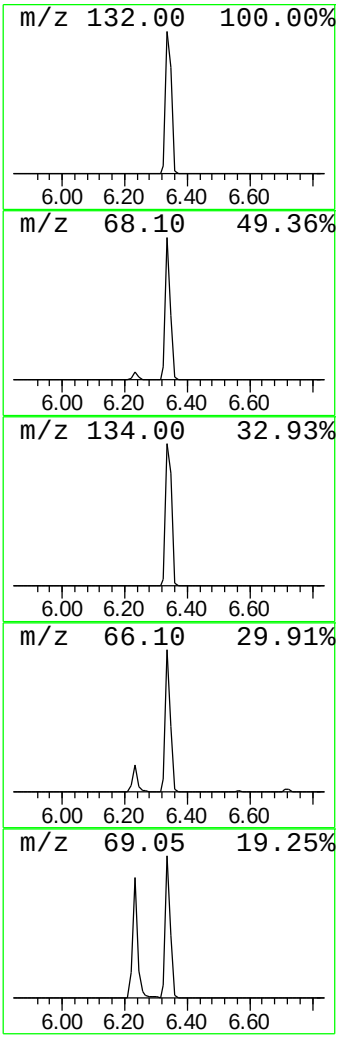
****

Peak Number 6 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	103.17 ng	5137090	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Xenon	132	Xe	007440-63-3	9





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Operator : UM/SJ
Sample : I1219-01
Misc :
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Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

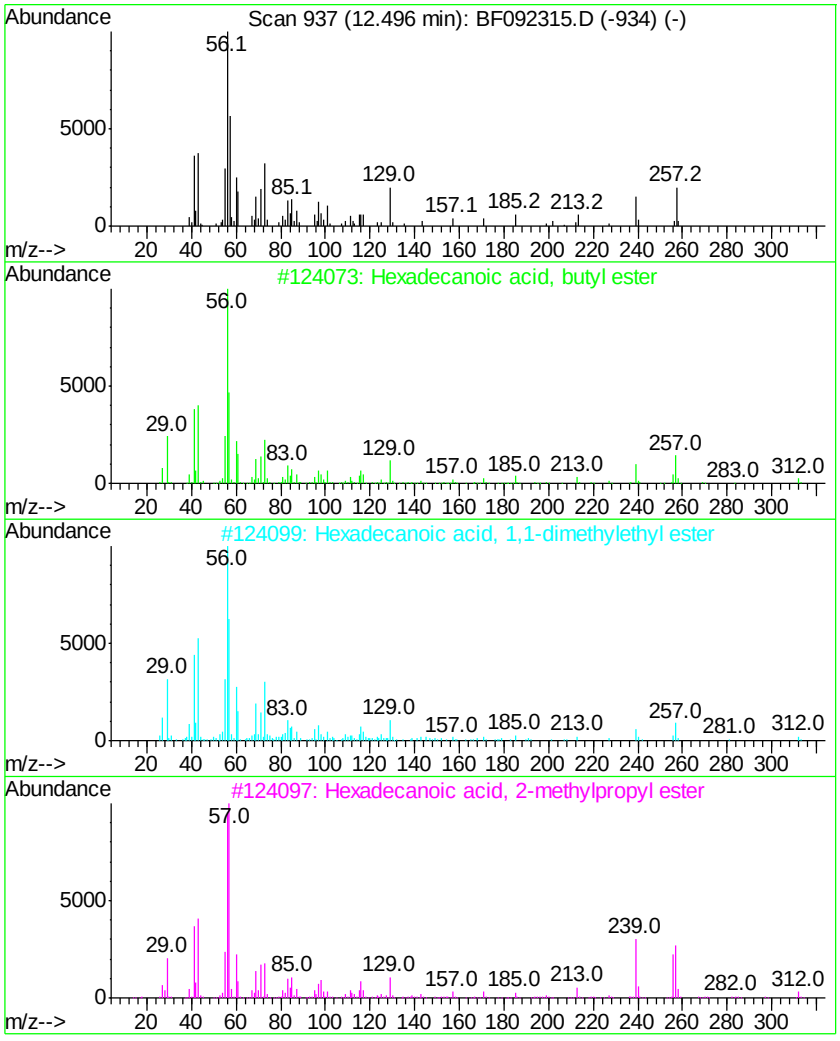
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

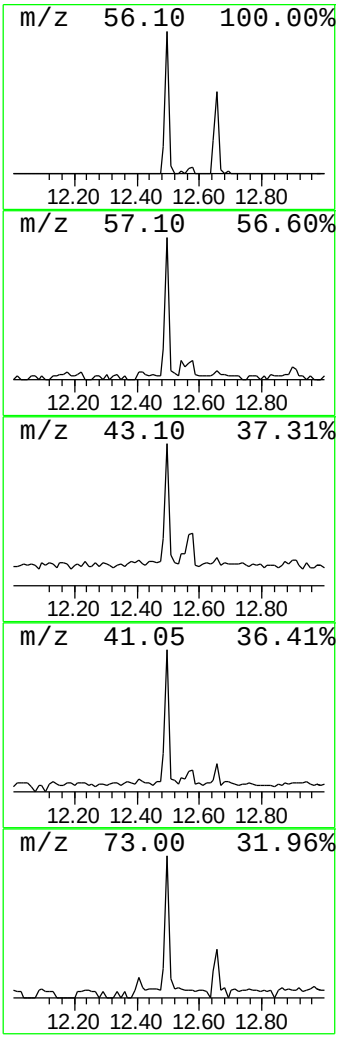
****

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	2.11 ng	121725	Chrysene-d12	13.70

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	74
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
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Operator : UM/SJ
Sample : I1219-01
Misc :
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Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

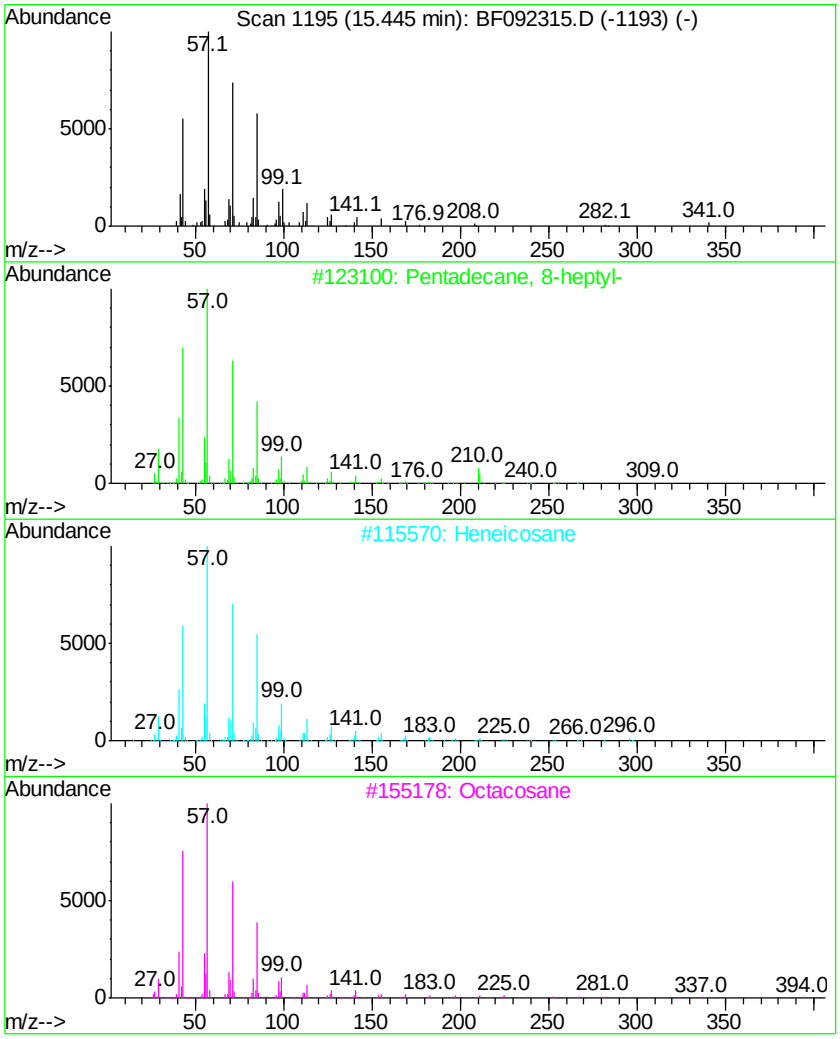
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

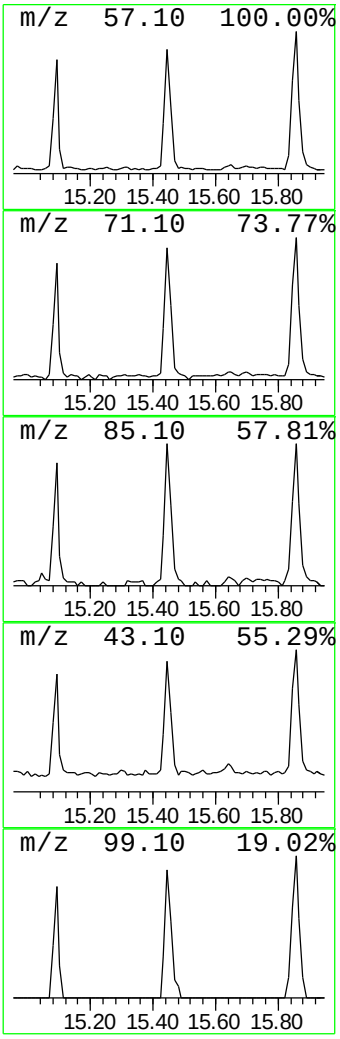
****

Peak Number 9 Pentadecane, 8-heptyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.23 ng	131908	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	Eicosane	282	C20H42	000112-95-8	86





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Sample : I1219-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

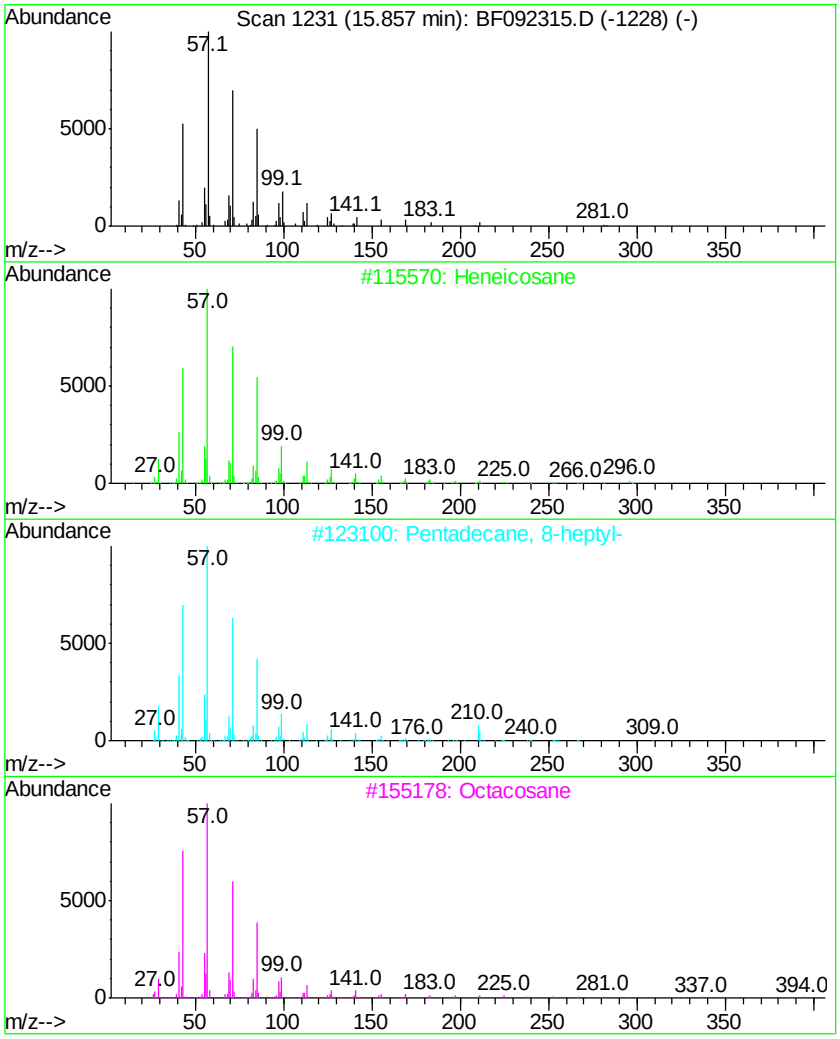
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

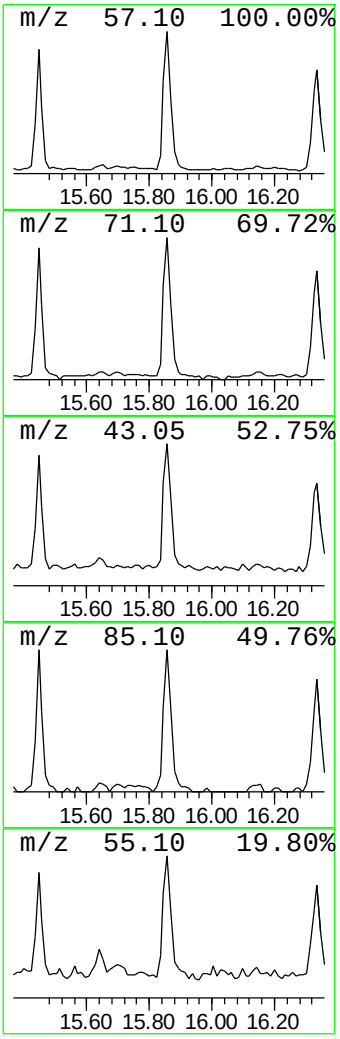
****

Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	3.08 ng	182084	Perylene-d12	15.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011617\
Data File : BF092315.D
Acq On : 17 Jan 2017 7:29
Operator : UM/SJ
Sample : I1219-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TOD-WCS-011317(11-47)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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
n-Propyl acetate	2.21	7.2	ng	358734	1	6.56	995898	20.0
4-Penten-2-one, 4...	2.85	5.6	ng	279147	1	6.56	995898	20.0
3-Penten-2-one, 4...	3.96	60.5	ng	3010770	1	6.56	995898	20.0
2-Pentanone, 4-hy...	4.70	40.3	ng	2004300	1	6.56	995898	20.0
unknown4.99	4.99	2.6	ng	130400	1	6.56	995898	20.0
unknown6.34	6.34	103.2	ng	5137090	1	6.56	995898	20.0
Hexadecanoic acid...	12.50	2.1	ng	121725	5	13.70	1156380	20.0
Pentadecane, 8-he...	15.45	2.2	ng	131908	6	15.06	1183670	20.0
Heneicosane	15.86	3.1	ng	182084	6	15.06	1183670	20.0