LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084659.D
Acq On : 30 Jan 2016 2:23
Operator : SJ/IZ
Sample : H1303-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM2-UST-21

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-BF012916.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	4.190	182	184	189	rBV	332490	432862	6.41%	0.698%
2	4.899	241	246	248	rBV	3024825	5359486	79.32%	8.640%
3	5.333	281	284	286	rBV	4175400	6126909	90.68%	9.877%
4	5.721	316	318	321	rBV	325398	333513	4.94%	0.538%
5	6.373	372	375	378	rBV	4809683	5358324	79.31%	8.638%
6	6.499	383	386	388	rBV	5478903	6422049	95.05%	10.353%
7	6.727	403	406	408	rBV	851619	1138220	16.85%	1.835%
8	6.876	417	419	422	rVB	3943933	4211325	62.33%	6.789%
9	7.287	452	455	458	rBV	2799807	4047939	59.91%	6.526%
10	7.402	461	465	472	rBV	52071	93668	1.39%	0.151%
11	8.007	516	518	520	rBV	1829137	1562494	23.13%	2.519%
12	9.093	610	613	615	rBV	6540496	6756566	100.00%	10.892%
13	9.482	645	647	650	rBV	757244	785085	11.62%	1.266%
14	9.699	665	666	669	rBV	76214	92264	1.37%	0.149%
15	9.756	669	671	674	rVB	1651097	1704812	25.23%	2.748%
16	10.202	709	710	712	rVB	210138	158880	2.35%	0.256%
17	10.419	726	729	732	rBV	81613	127621	1.89%	0.206%
18	10.545	738	740	743	rBV2	3426551	4505640	66.69%	7.264%
19	10.671	750	751	756	rBV	202251	278155	4.12%	0.448%
20	11.116	788	790	792	rBV	108721	132618	1.96%	0.214%
21	11.242	798	801	803	rBV	1584507	1764989	26.12%	2.845%
22	11.791	846	849	851	rBV	136401	154455	2.29%	0.249%
23	12.831	937	940	942	rBV	6281825	6579661	97.38%	10.607%
24	13.745	1017	1020	1028	rBV	194790	600228	8.88%	0.968%
25	13.871	1028	1031	1033	rVB	1805146	1823019	26.98%	2.939%
26	14.717	1103	1105	1108	rBV	103874	94710	1.40%	0.153%
27	15.254	1149	1152	1155	rBV	1102751	1293780	19.15%	2.086%
28	15.791	1195	1199	1205	rBV8	21832	90635	1.34%	0.146%

Sum of corrected areas: 62029907

LSC Report - Integrated Chromatogram

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Data File : BF084659.D
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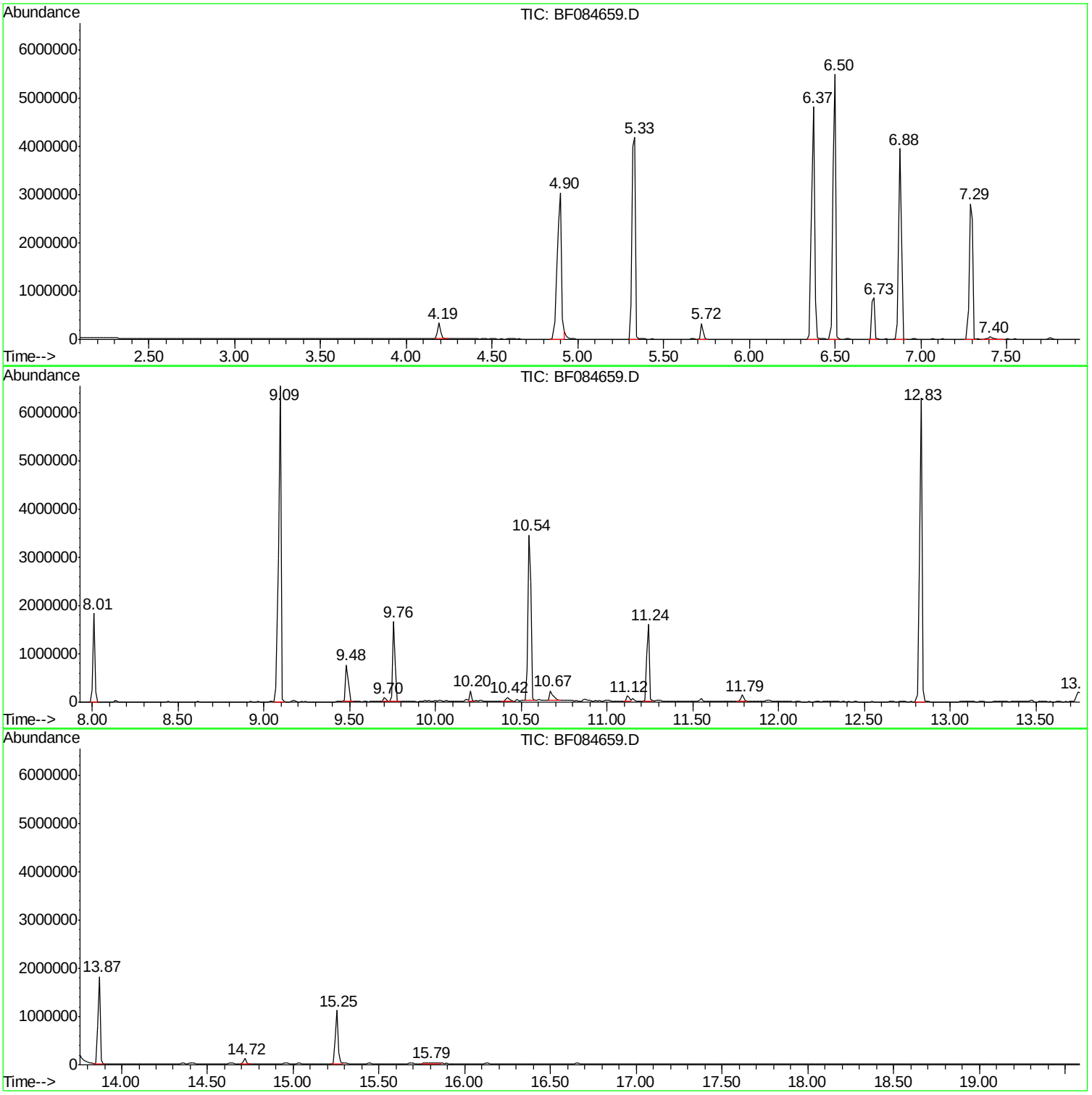
Operator : SJ/IZ
Sample : H1303-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM2-UST-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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\BF012916\
Data File : BF084659.D
Acq On : 30 Jan 2016 2:23
Operator : SJ/IZ
Sample : H1303-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM2-UST-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

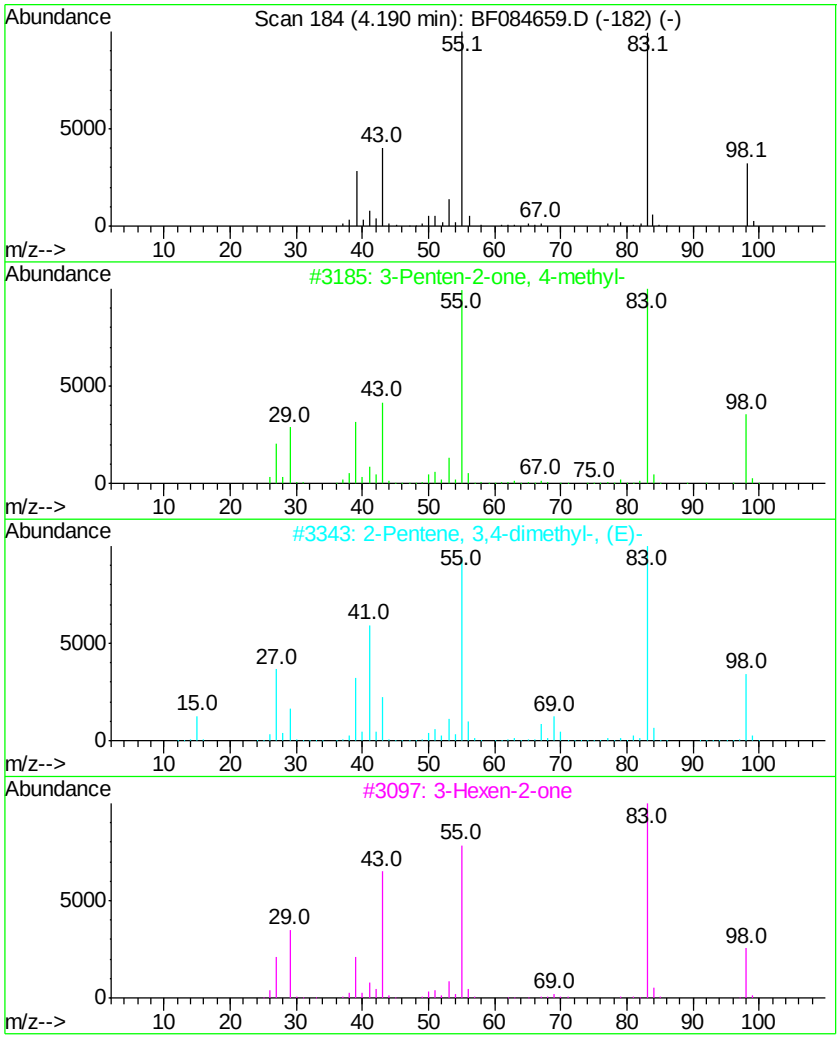
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

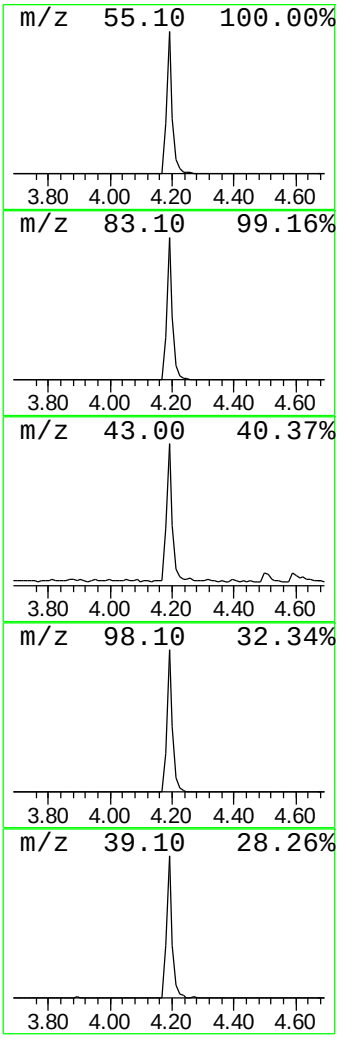
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	7.61 ng	432862	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	90
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





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Data File : BF084659.D
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Sample : H1303-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM2-UST-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

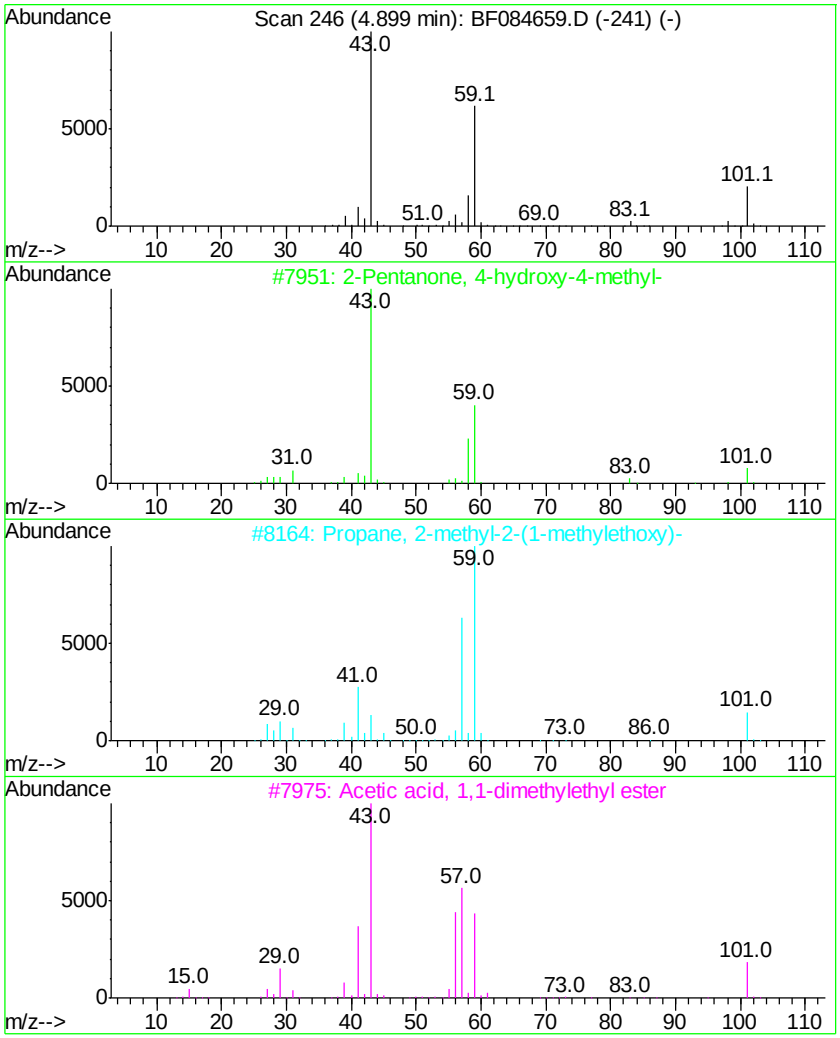
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

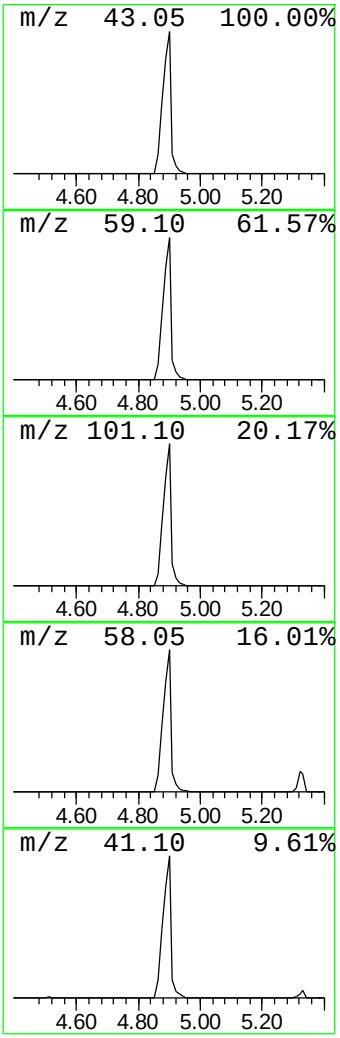
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	94.17 ng	5359490	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084659.D
Acq On : 30 Jan 2016 2:23
Operator : SJ/IZ
Sample : H1303-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM2-UST-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

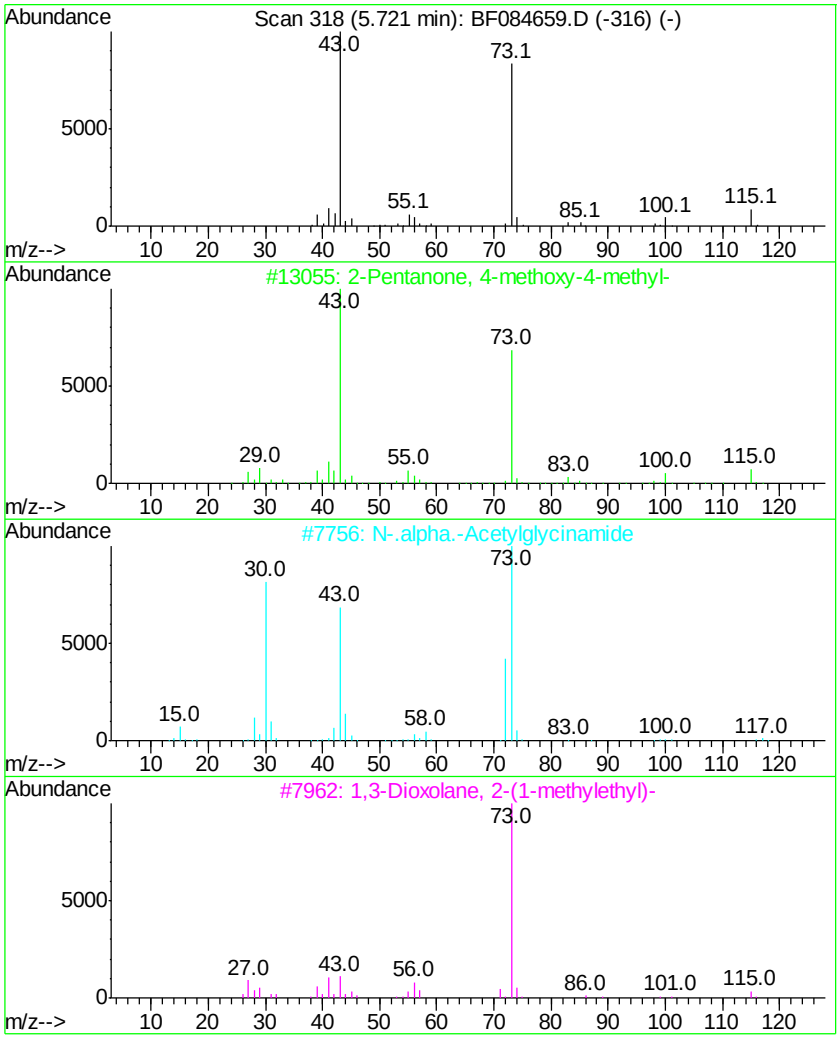
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

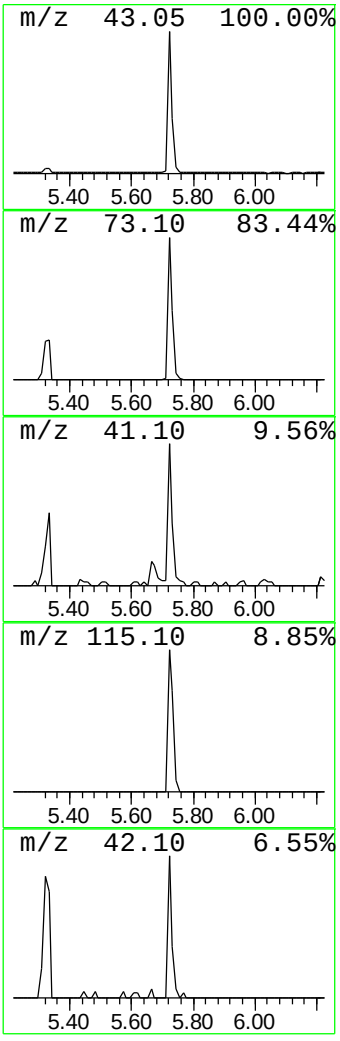
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	5.86 ng	333513	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	43
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084659.D
Acq On : 30 Jan 2016 2:23
Operator : SJ/IZ
Sample : H1303-08
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM2-UST-21

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

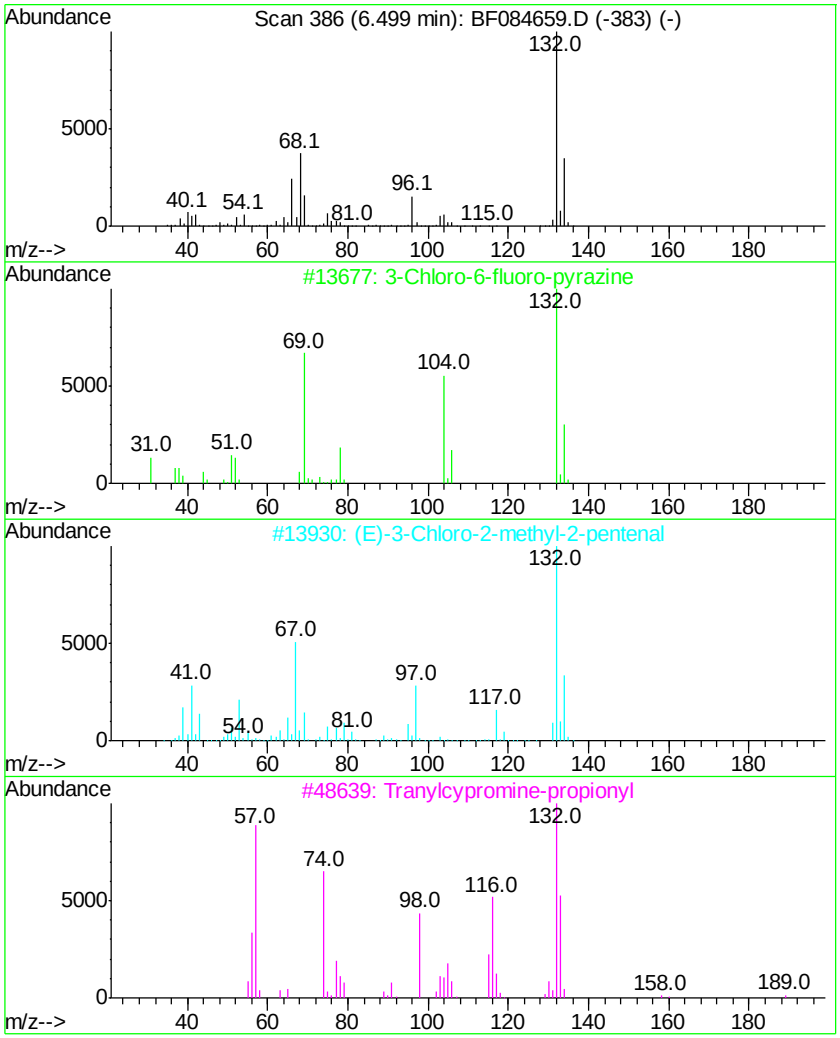
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

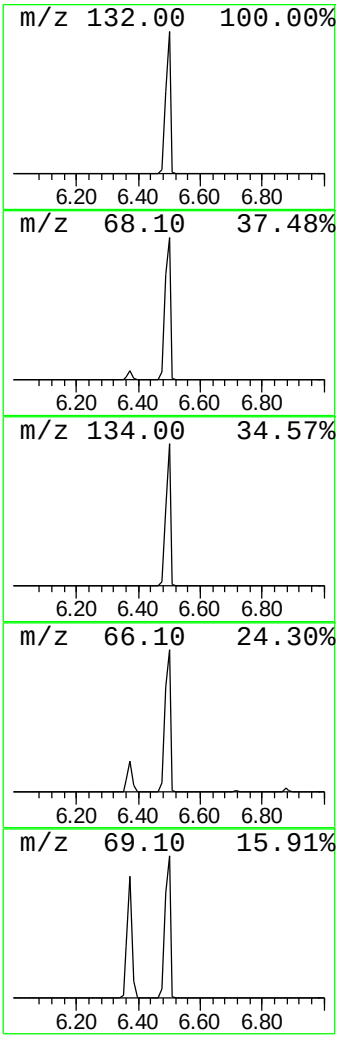
****

Peak Number 4 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	112.84 ng	6422050	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
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Sample : H1303-08
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ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BOTTOM2-UST-21

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TIC Library : C:\DATABASE\NIST02.L
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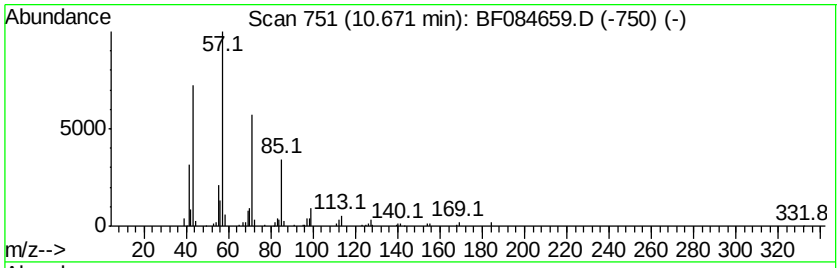
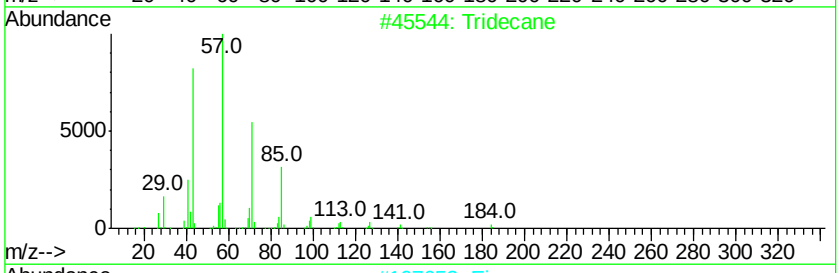
****

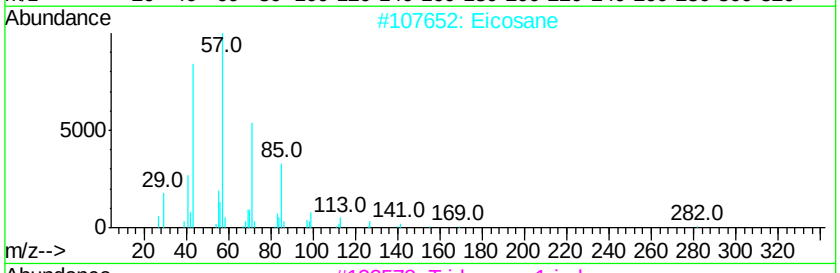
Peak Number 6 Tridecane Concentration Rank 7

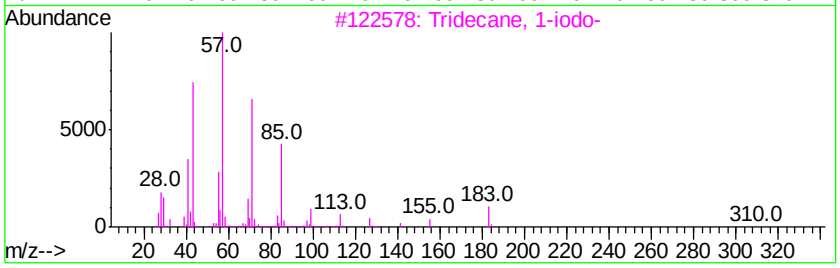
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	3.15 ng	278155	Phenanthrene-d10	11.24

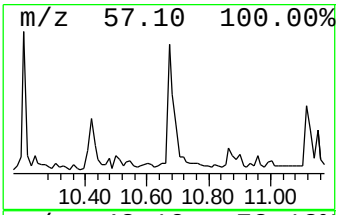
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Tetradecane	198	C14H30	000629-59-4	90

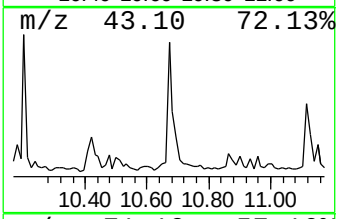


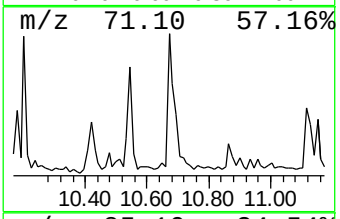


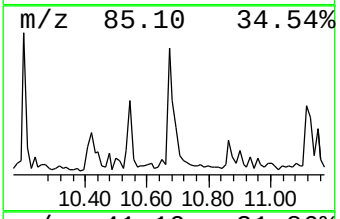


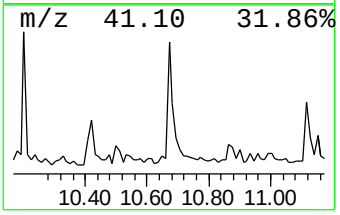












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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

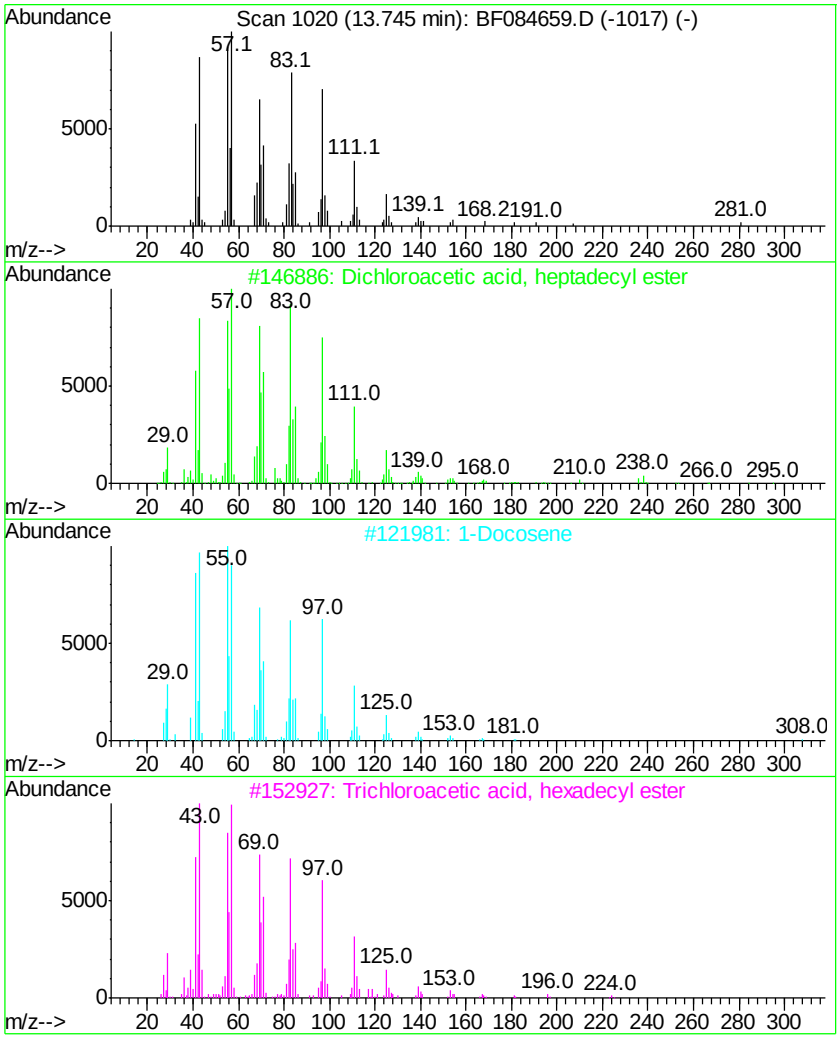
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

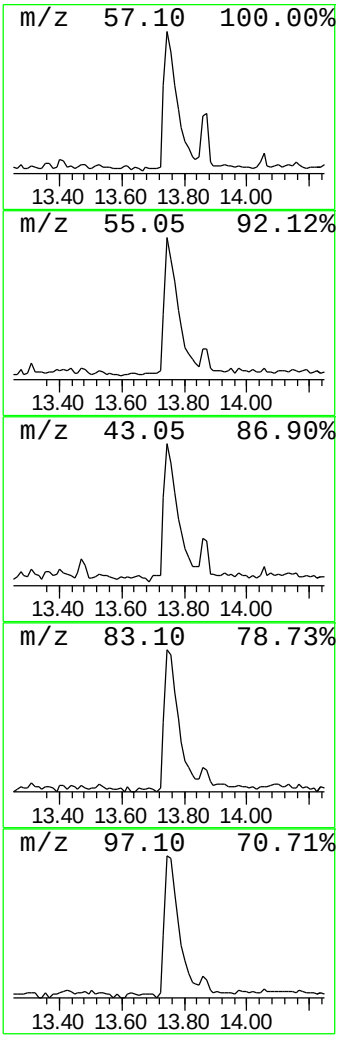
****

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	6.58 ng	600228	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	11-Tricosene	322	C23H46	052078-56-5	91
5	1-Nonadecanol	284	C19H40O	001454-84-8	91





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...	4.19	7.6	ng	432862	1	6.73	1138220	20.0
2-Pentanone, 4-hy...	4.90	94.2	ng	5359490	1	6.73	1138220	20.0
2-Pentanone, 4-me...	5.72	5.9	ng	333513	1	6.73	1138220	20.0
unknown6.50	6.50	112.8	ng	6422050	1	6.73	1138220	20.0
Tridecane	10.67	3.1	ng	278155	4	11.24	1764990	20.0
Dichloroacetic ac...	13.75	6.6	ng	600228	5	13.87	1823020	20.0