LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101072.D
Acq On : 1 Dec 2017 19:18
Operator : SJ/JU
Sample : I6622-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1A-2-4

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-BF113017.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	5.081	506	509	524	rVB	58748	85649	5.89%	0.697%
2	5.475	571	576	579	rBV	1315195	1378788	94.83%	11.223%
3	6.486	742	748	756	rBV	1312861	1454028	100.00%	11.835%
4	6.622	766	771	774	rBV	1591454	1446256	99.47%	11.772%
5	6.845	806	809	813	rBV	379502	308104	21.19%	2.508%
6	7.004	832	836	839	rBV	1240790	1078444	74.17%	8.778%
7	7.416	901	906	909	rBV	924870	866402	59.59%	7.052%
8	8.128	1024	1027	1031	rBV	478680	390778	26.88%	3.181%
9	9.204	1206	1210	1213	rBV	1694722	1417580	97.49%	11.538%
10	9.275	1219	1222	1225	rBB	20569	16253	1.12%	0.132%
11	9.598	1273	1277	1280	rBV	128383	109677	7.54%	0.893%
12	9.804	1309	1312	1317	rVB	36286	27237	1.87%	0.222%
13	9.886	1322	1326	1329	rVV	477022	403515	27.75%	3.284%
14	10.304	1394	1397	1400	rVB	33994	26832	1.85%	0.218%
15	10.674	1456	1460	1464	rBV	803298	690241	47.47%	5.618%
16	10.780	1475	1478	1487	rVB	26242	32032	2.20%	0.261%
17	11.374	1575	1579	1581	rBV	403936	340328	23.41%	2.770%
18	11.398	1581	1583	1586	rVB	42188	33754	2.32%	0.275%
19	12.586	1782	1785	1789	rVB	71918	57081	3.93%	0.465%
20	12.815	1818	1824	1827	rBV	64213	61978	4.26%	0.504%
21	12.957	1844	1848	1851	rBV	1104555	990229	68.10%	8.060%
22	13.145	1874	1880	1884	rBV2	13794	21039	1.45%	0.171%
23	13.457	1930	1933	1937	rVB	28040	22086	1.52%	0.180%
24	13.839	1995	1998	2005	rVB3	104770	125108	8.60%	1.018%
25	14.015	2023	2028	2031	rBV	404136	371963	25.58%	3.028%
26	14.039	2031	2032	2035	rVB	37637	24708	1.70%	0.201%
27	14.474	2103	2106	2109	rBV3	14347	19139	1.32%	0.156%
28	14.757	2151	2154	2162	rBV	65476	79974	5.50%	0.651%
29	15.057	2201	2205	2208	rBV	38092	51578	3.55%	0.420%
30	15.362	2254	2257	2260	rVB2	20942	21700	1.49%	0.177%
31	15.421	2264	2267	2271	rVB	25364	30969	2.13%	0.252%
32	15.486	2273	2278	2283	rBV	213958	281845	19.38%	2.294%
33	15.974	2357	2361	2364	rBV5	12672	20554	1.41%	0.167%

LSC Area Percent Report

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Data File : BF101072.D
Acq On : 1 Dec 2017 19:18
Operator : SJ/JU
Sample : I6622-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1A-2-4

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 12285849

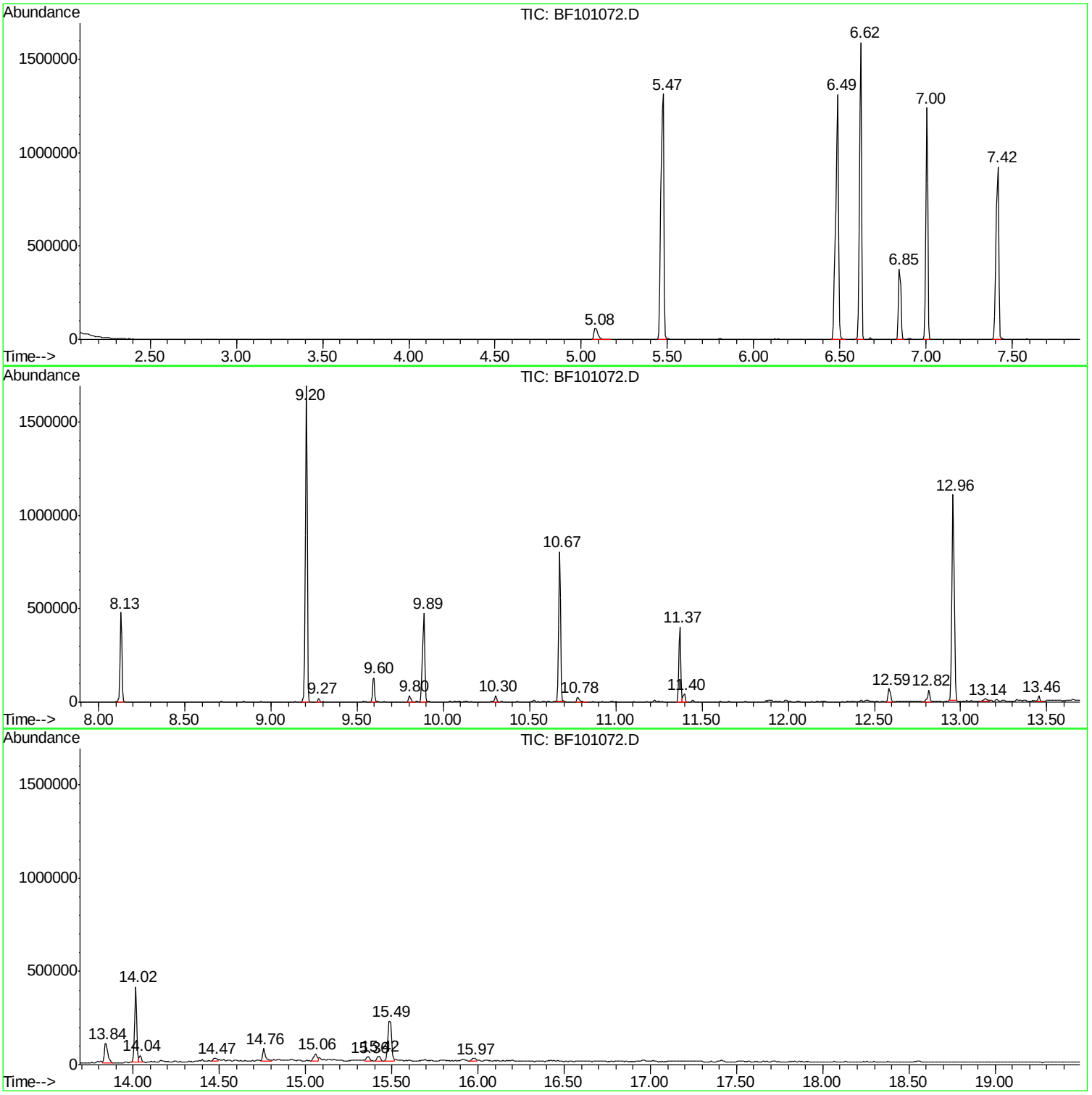
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101072.D
Acq On : 1 Dec 2017 19:18
Operator : SJ/JU
Sample : I6622-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1A-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101072.D
Acq On : 1 Dec 2017 19:18
Operator : SJ/JU
Sample : I6622-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1A-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

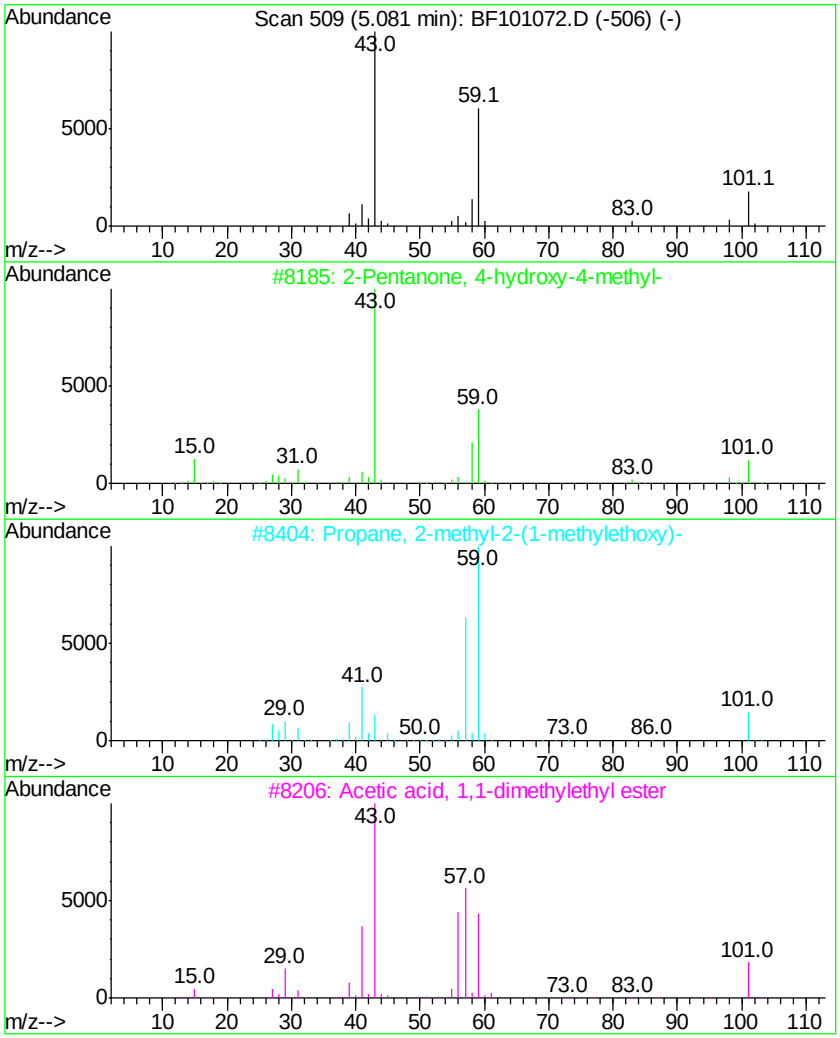
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

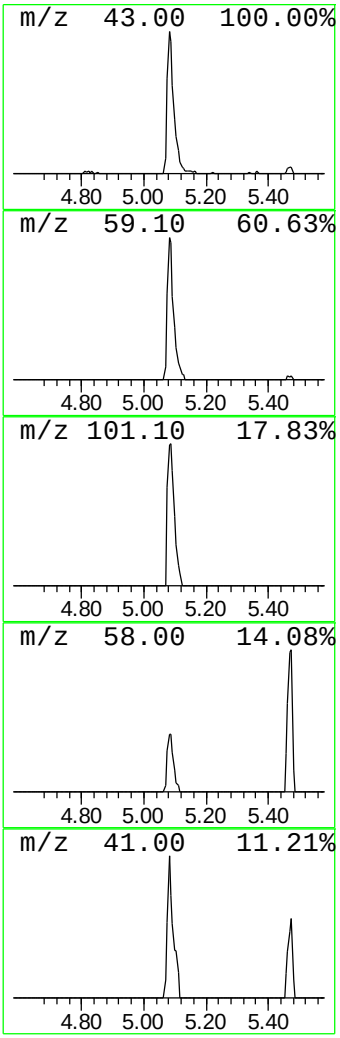
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	5.56 ng	85649	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF120117\
Data File : BF101072.D
Acq On : 1 Dec 2017 19:18
Operator : SJ/JU
Sample : I6622-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1A-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

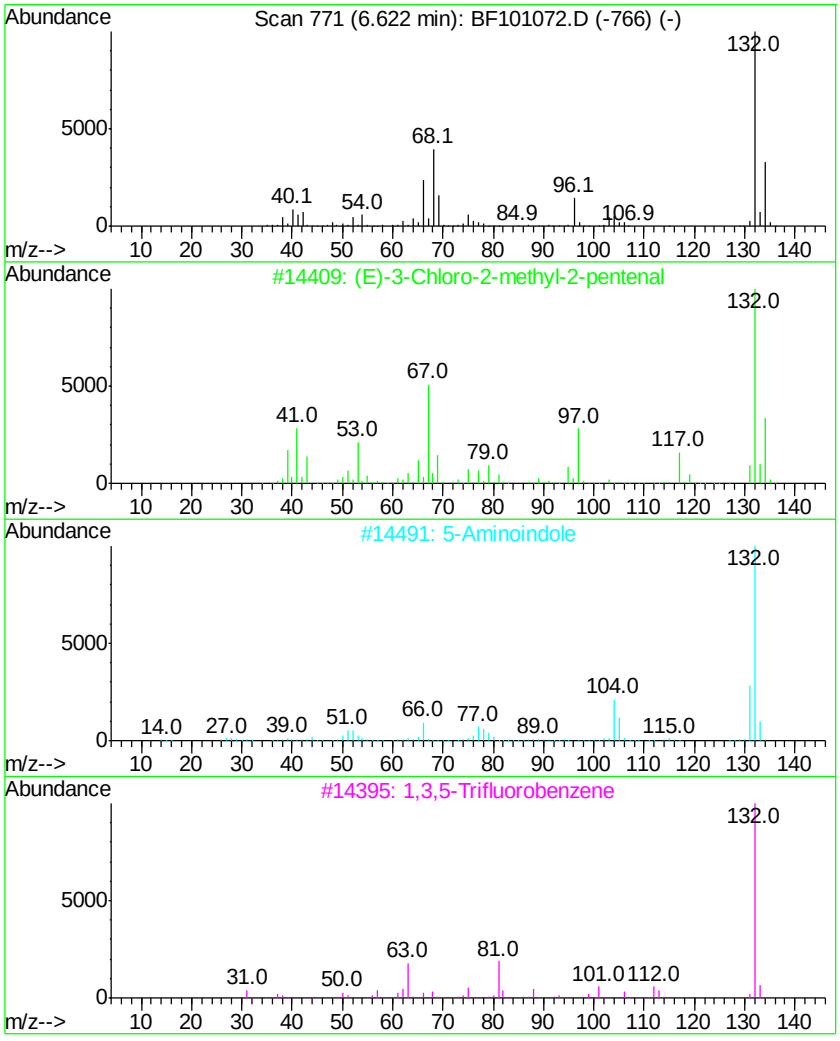
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

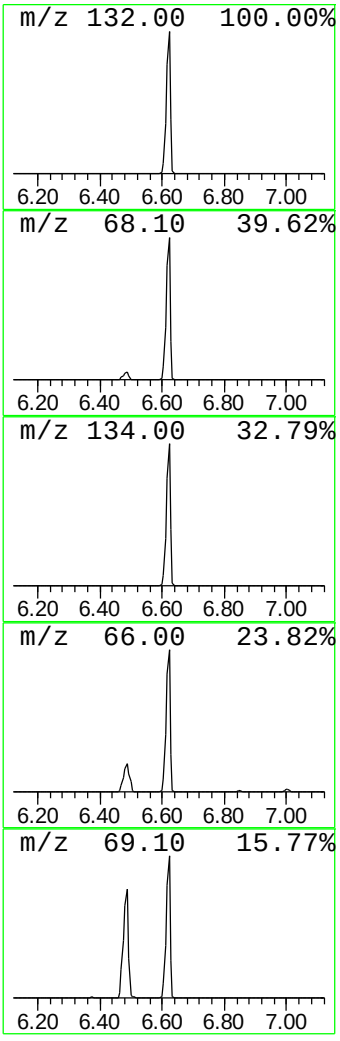
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	93.88 ng	1446260	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Data File : BF101072.D
Acq On : 1 Dec 2017 19:18
Operator : SJ/JU
Sample : I6622-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1A-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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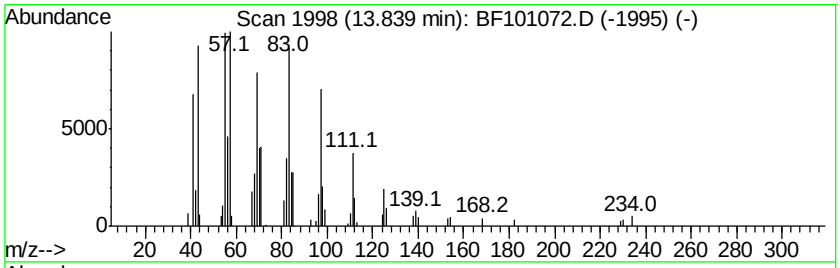
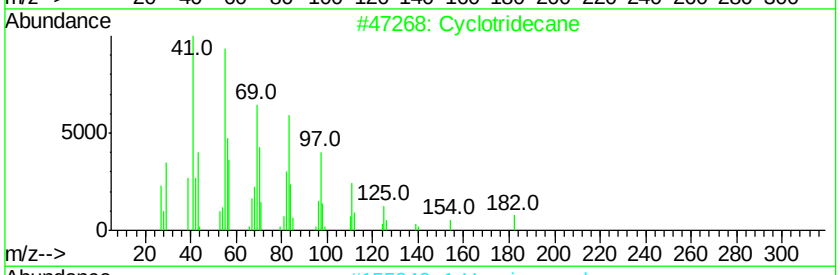
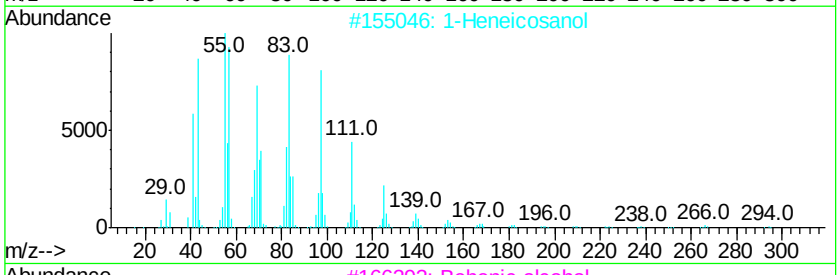
Peak Number 4 Cyclotridecane Concentration Rank 3

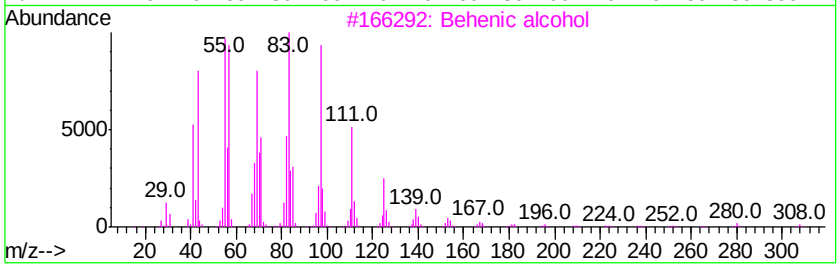
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	6.73 ng	125108	Chrysene-d12	14.02

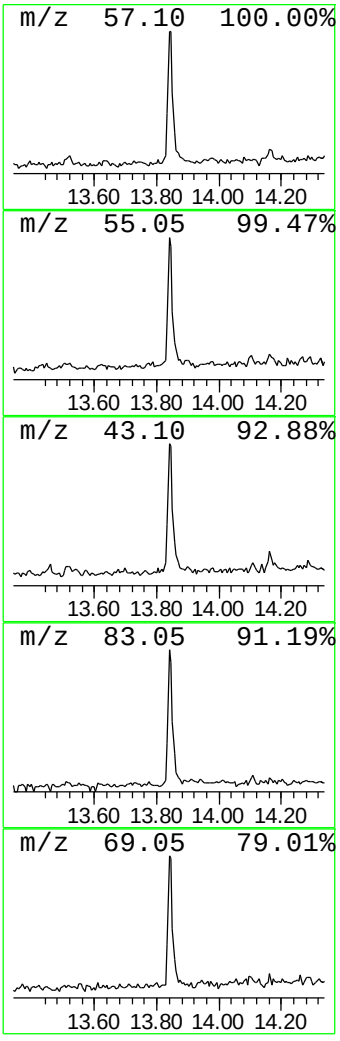
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotridecane	182	C13H26	000295-02-3	97
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	95











Library Search Compound Report

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBNW1A-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

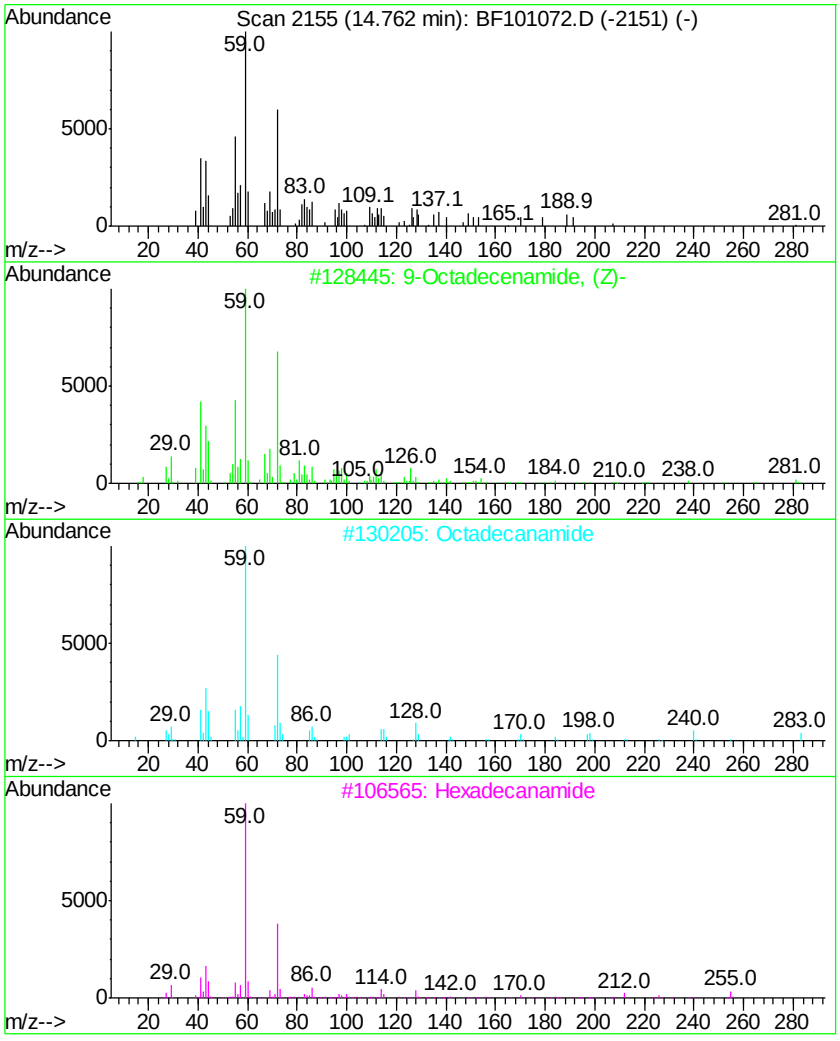
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

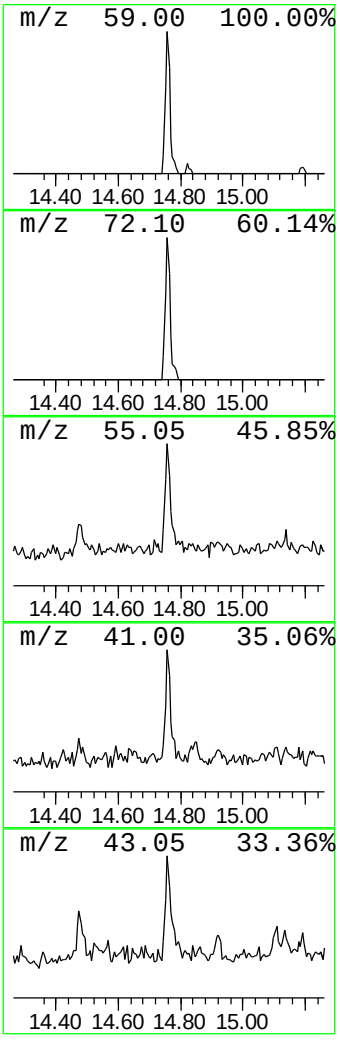
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	5.68 ng	79974	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Octadecanamide	283	C18H37NO	000124-26-5	59
3	Hexadecanamide	255	C16H33NO	000629-54-9	59
4	Tetradecanamide	227	C14H29NO	000638-58-4	50
5	Dodecanamide	199	C12H25NO	001120-16-7	50





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF120117\
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	5.6	ng	85649	1	6.85	308104	20.0
unknown6.62	6.62	93.9	ng	1446260	1	6.85	308104	20.0
Cyclotridecane	13.84	6.7	ng	125108	5	14.02	371963	20.0
9-Octadecenamide,...	14.76	5.7	ng	79974	6	15.49	281845	20.0