LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
Data File : BM009995.D
Acq On : 11 May 2017 21:30
Operator : SJ/MA
Sample : I3058-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW003-170508

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_M\METHODS\8270-BM051117.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	4.899	303	308	317	rBV	154569	234232	3.01%	0.720%
2	5.351	379	385	399	rBV	966444	1447989	18.61%	4.453%
3	5.463	399	404	416	rVB	180766	280546	3.61%	0.863%
4	6.946	649	656	672	rBV	611906	1027262	13.20%	3.159%
5	7.298	708	716	730	rBV	1723406	2683888	34.50%	8.253%
6	7.763	789	795	804	rBV	293278	474233	6.10%	1.458%
7	8.081	841	849	857	rBV	1325271	2126437	27.33%	6.539%
8	8.934	986	994	1008	rBV	1271667	2207636	28.37%	6.789%
9	10.557	1262	1270	1278	rBV	367130	643592	8.27%	1.979%
10	13.027	1683	1690	1699	rBV	3044135	4422894	56.85%	13.600%
11	13.880	1829	1835	1844	rBV	98202	148413	1.91%	0.456%
12	14.416	1920	1926	1936	rVB2	563670	873765	11.23%	2.687%
13	15.169	2046	2054	2063	rBV2	46515	78870	1.01%	0.243%
14	15.916	2175	2181	2198	rBV	2726889	3922237	50.41%	12.061%
15	17.174	2386	2395	2403	rBV	767998	1134662	14.58%	3.489%
16	17.545	2452	2458	2466	rBV4	119962	220039	2.83%	0.677%
17	18.915	2684	2691	2696	rBV2	112602	171637	2.21%	0.528%
18	19.798	2835	2841	2846	rBV	6775277	7780407	100.00%	23.925%
19	21.050	3050	3054	3061	rBV7	62153	103729	1.33%	0.319%
20	21.362	3102	3107	3116	rBV	1084922	1417809	18.22%	4.360%
21	23.656	3490	3497	3506	rBV2	539496	1119921	14.39%	3.444%

Sum of corrected areas: 32520198

LSC Report - Integrated Chromatogram

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Data File : BM009995.D
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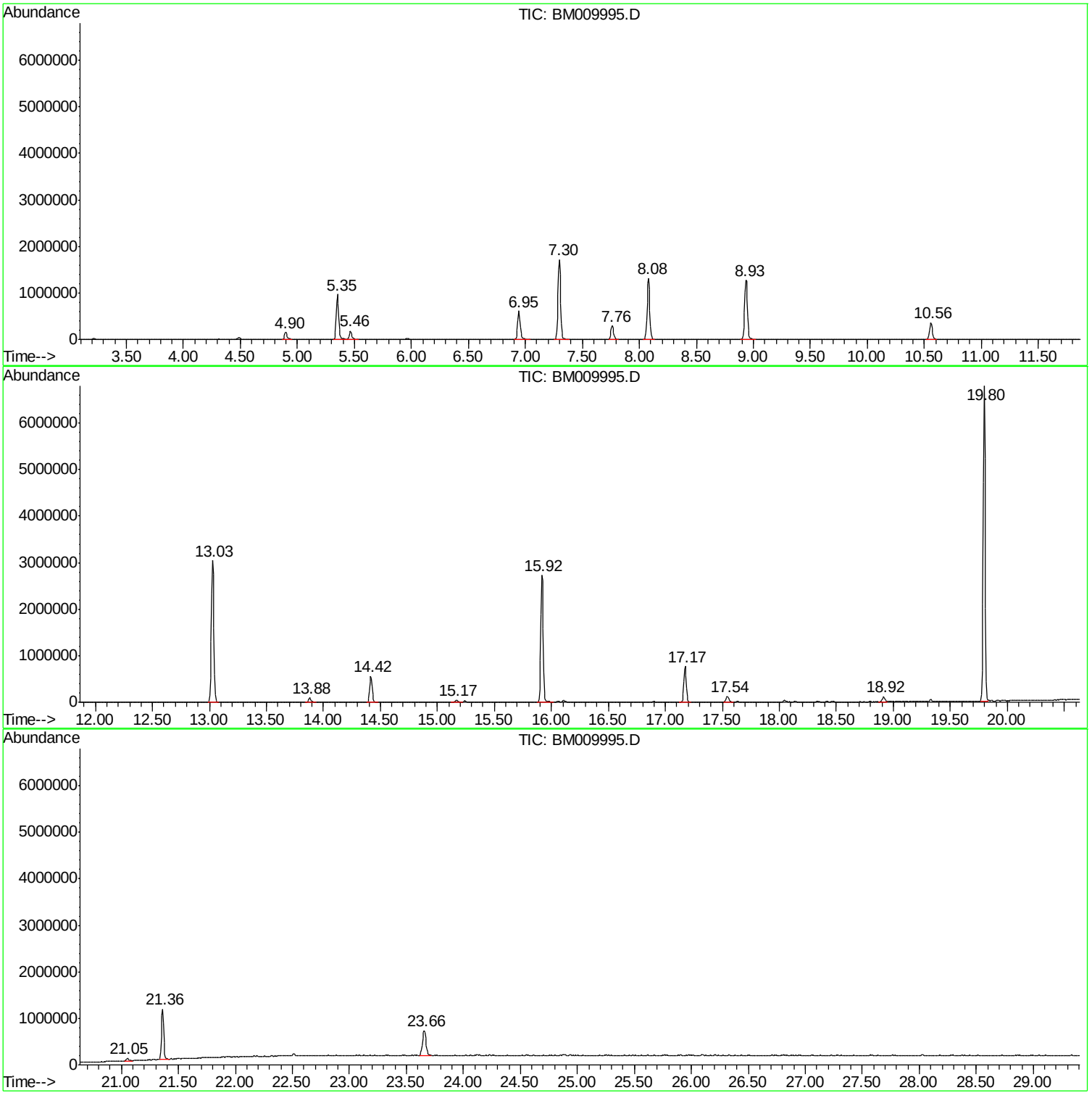
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LF017MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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 M\DATA\BM051117\
Data File : BM009995.D
Acq On : 11 May 2017 21:30
Operator : SJ/MA
Sample : I3058-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW003-170508

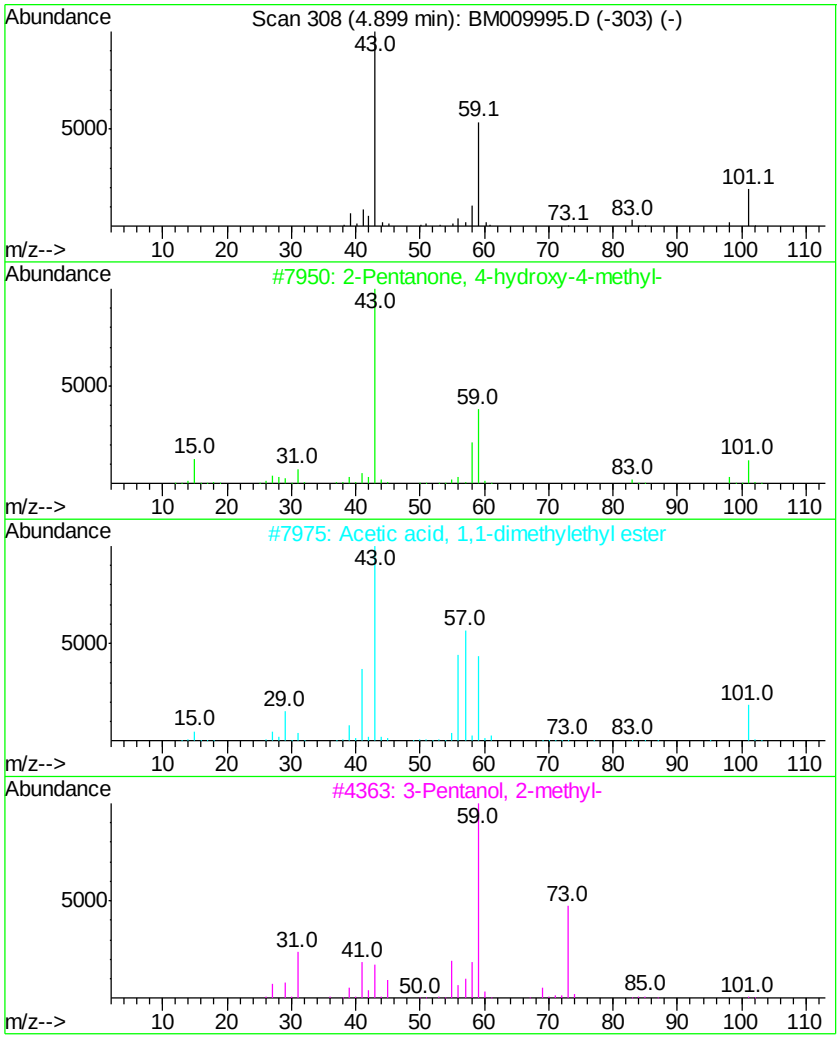
Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

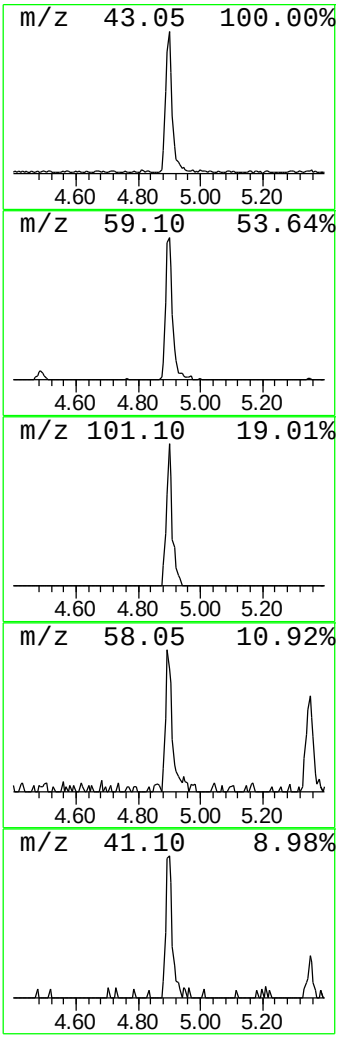
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	9.88 ng	234232	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	28
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Data File : BM009995.D
Acq On : 11 May 2017 21:30
Operator : SJ/MA
Sample : I3058-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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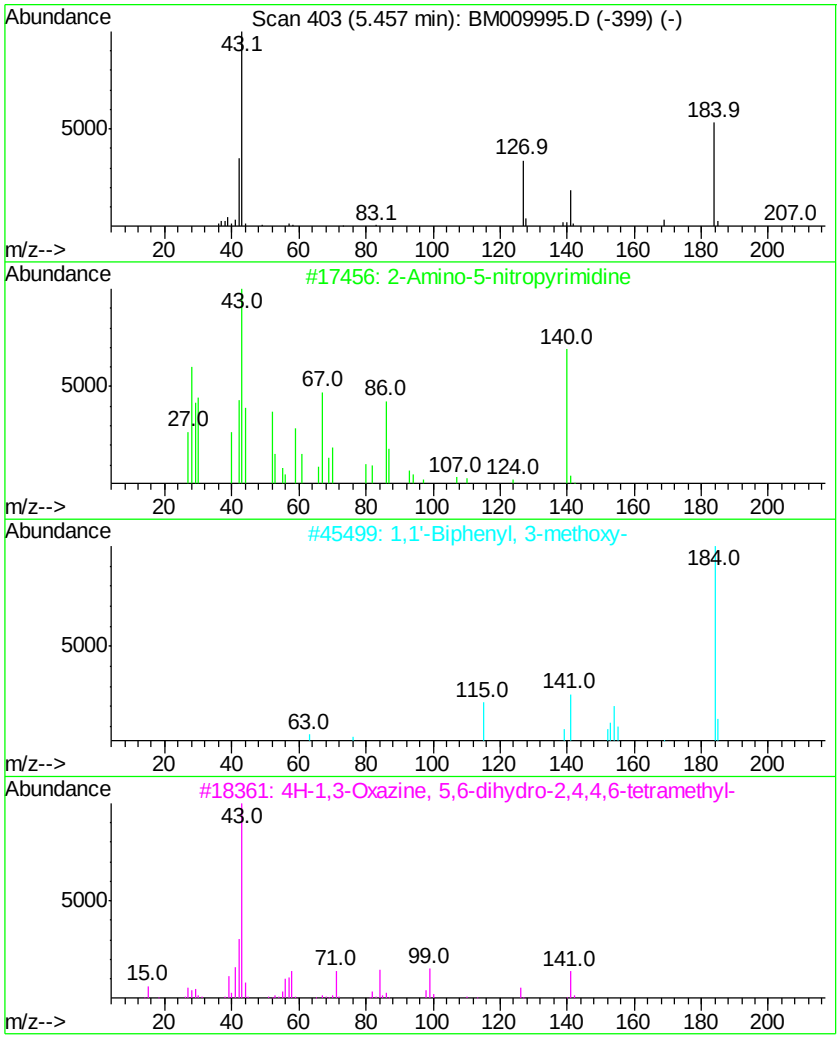
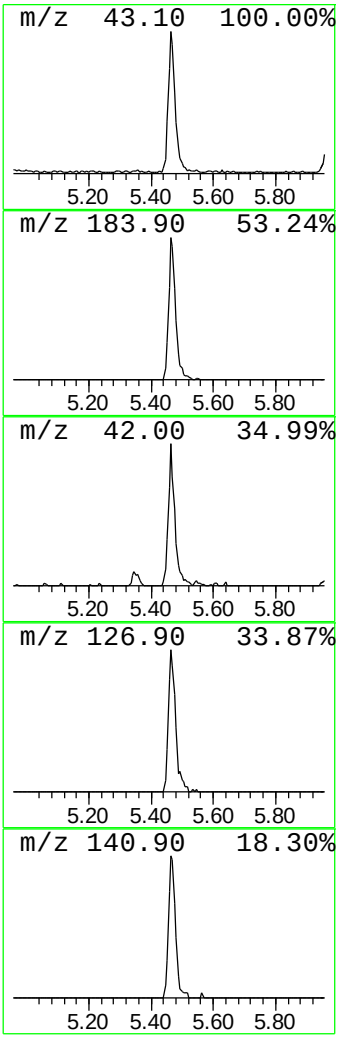
****

Peak Number 2 unknown5.46 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.46	11.83 ng	280546	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-5-nitropyrimidine	140	C4H4N4O2	003073-77-6	9
2	1,1'-Biphenyl, 3-methoxy-	184	C13H12O	002113-56-6	9
3	4H-1,3-Oxazine, 5,6-dihydro-2,4,...	141	C8H15NO	026939-18-4	9
4	.alpha.-D-Glucopyranoside, methy...	418	C20H34O9	1000157-04-1	9
5	1,1'-Biphenyl, 4-methoxy-	184	C13H12O	000613-37-6	7





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\
Data File : BM009995.D
Acq On : 11 May 2017 21:30
Operator : SJ/MA
Sample : I3058-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

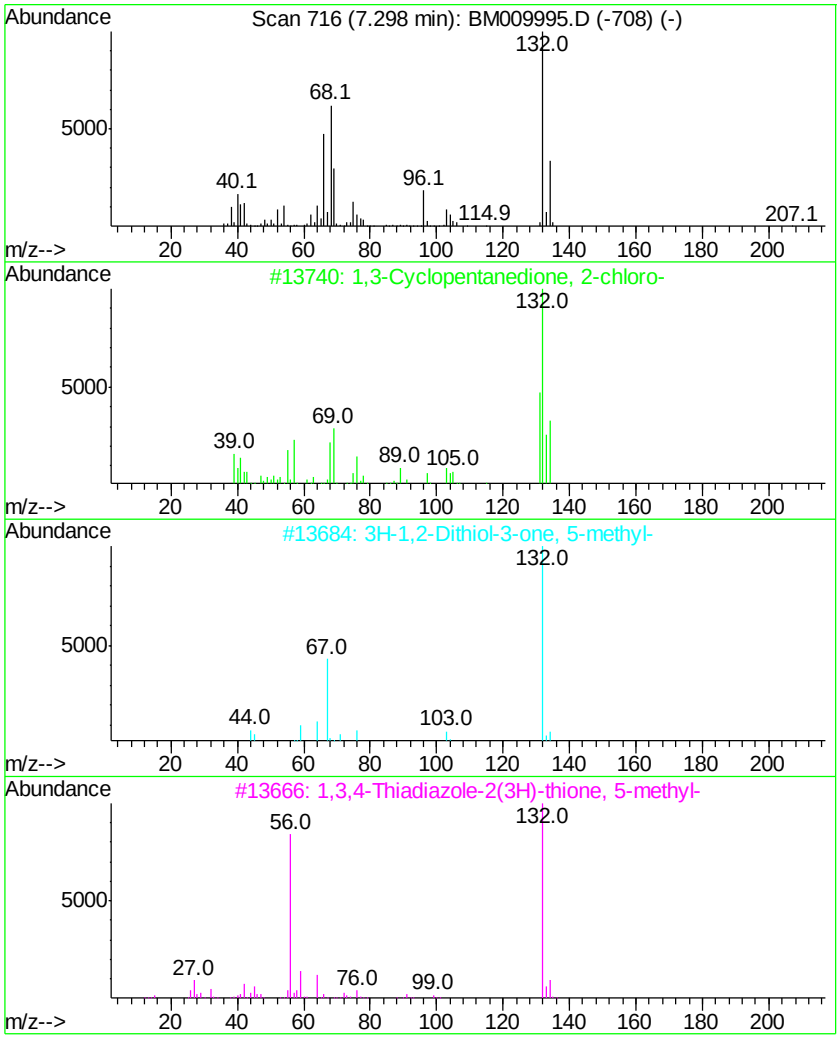
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

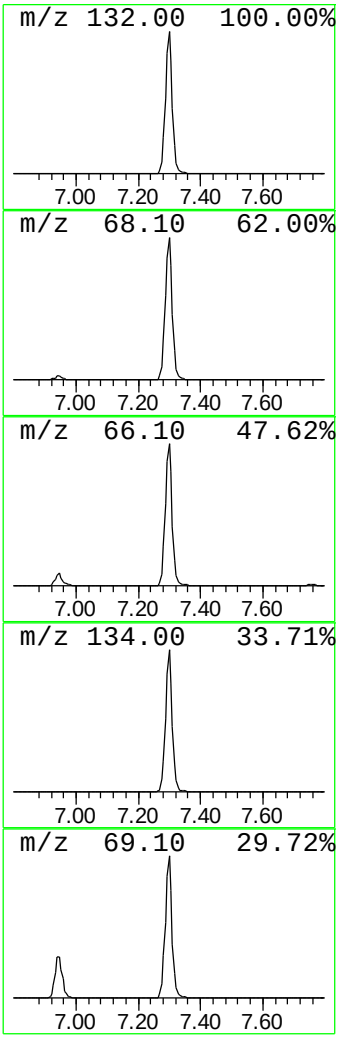
****

Peak Number 3 unknown7.30 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	113.19 ng	2683890	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	27
2	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14





Library Search Compound Report

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Data File : BM009995.D
Acq On : 11 May 2017 21:30
Operator : SJ/MA
Sample : I3058-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LF017MW003-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

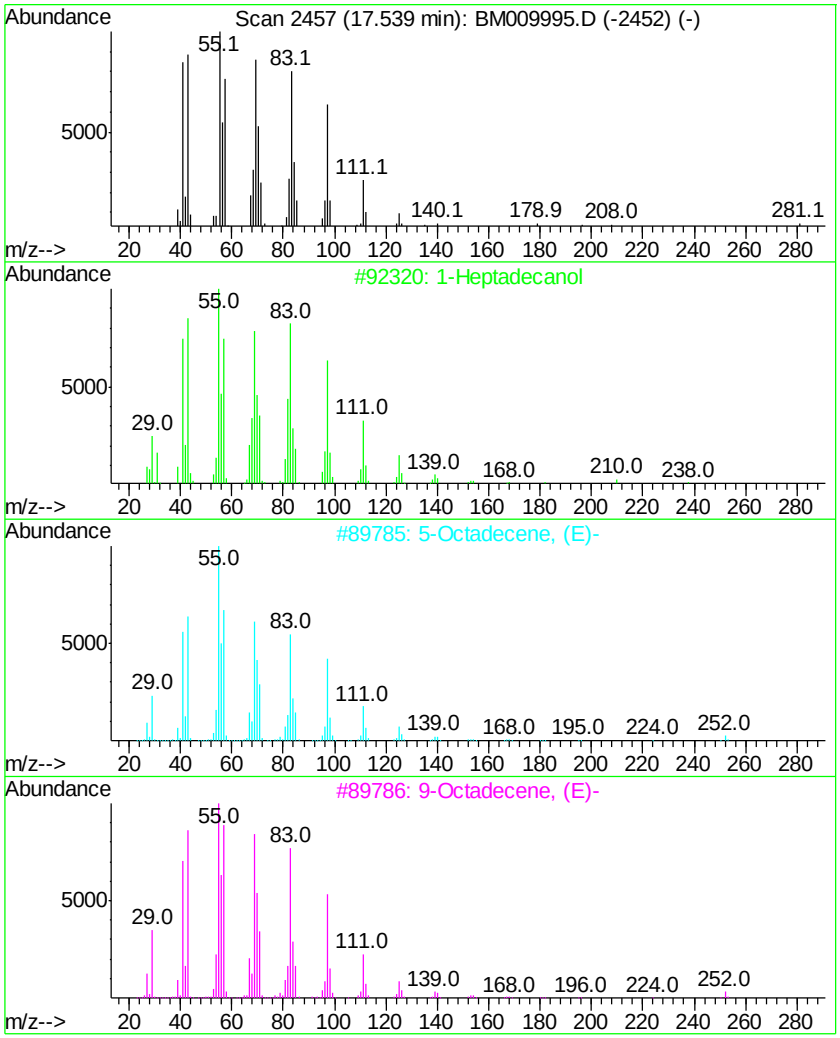
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

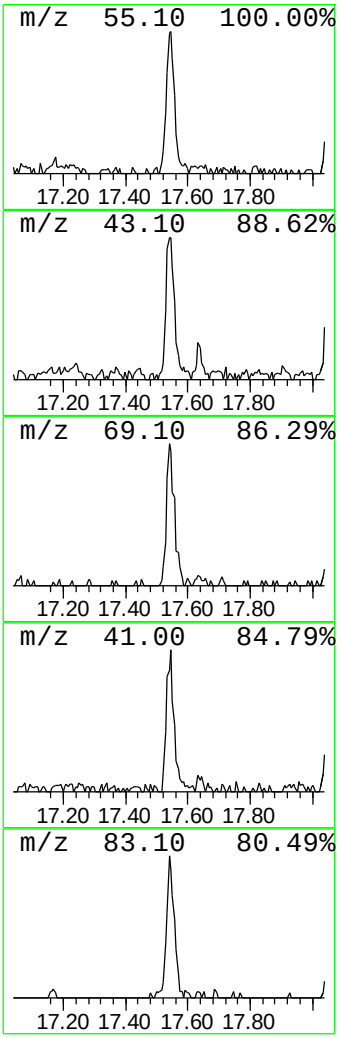
****

Peak Number 5 1-Heptadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.54	3.88 ng	220039	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecanol	256	C17H36O	001454-85-9	87
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	81
3	9-Octadecene, (E)-	252	C18H36	007206-25-9	81
4	1-Hexadecanol	242	C16H34O	036653-82-4	81
5	1-Tridecanol	200	C13H28O	000112-70-9	81





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Sample : I3058-08
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Instrument : BNA_M
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.M
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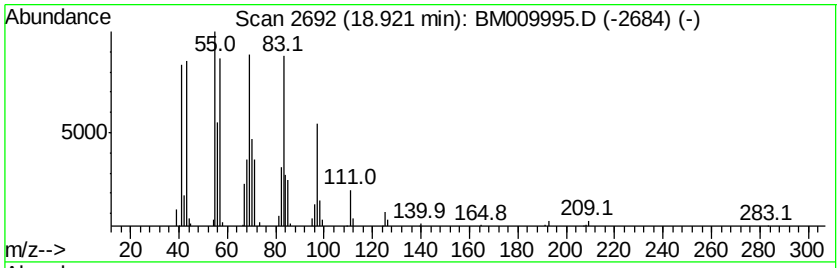
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

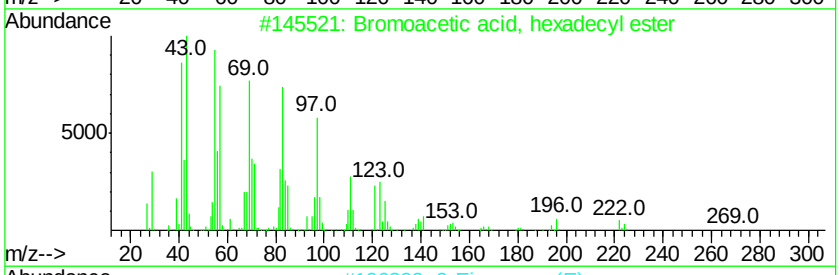
****

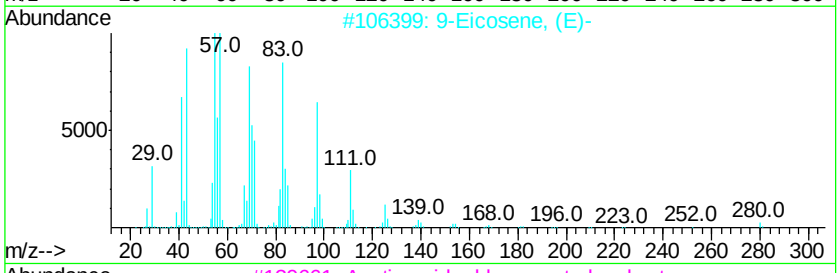
Peak Number 6 Bromoacetic acid, hexadecyl... Concentration Rank 6

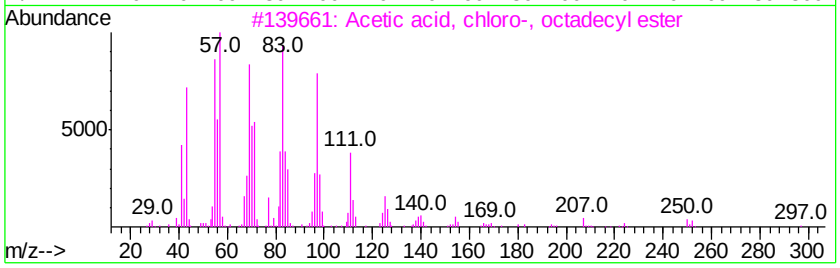
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.92	3.03 ng	171637	Phenanthrene-d10	17.17

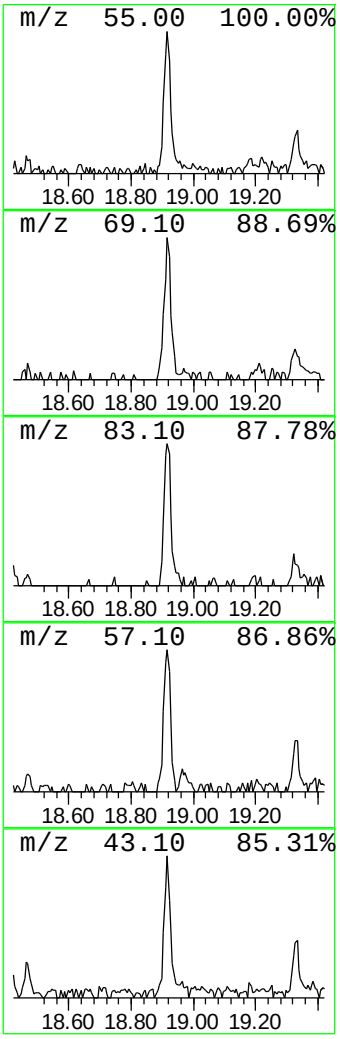
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
4	1-Nonadecanol	284	C19H40O	001454-84-8	91
5	1-Heptadecanol	256	C17H36O	001454-85-9	91











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051117\
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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
2-Pentanone, 4-hy...	4.90	9.9	ng	234232	1	7.76	474233	20.0
unknown5.46	5.46	11.8	ng	280546	1	7.76	474233	20.0
unknown7.30	7.30	113.2	ng	2683890	1	7.76	474233	20.0
1-Heptadecanol	17.54	3.9	ng	220039	4	17.17	1134660	20.0
Bromoacetic acid,...	18.92	3.0	ng	171637	4	17.17	1134660	20.0