LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EASTWALL-120116

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-BF112916.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	2.481	15	17	27	rVB	72900	126668	3.07%	0.309%
2	3.178	77	78	95	rBV4	21389	74109	1.80%	0.181%
3	5.041	238	241	247	rVB	1145939	1507804	36.56%	3.678%
4	5.453	274	277	279	rBV	2727963	3474751	84.25%	8.476%
5	6.481	364	367	370	rBV	2847871	3570596	86.57%	8.710%
6	6.619	377	379	382	rBV	2693997	3480338	84.38%	8.490%
7	6.859	398	400	402	rBV	1463545	1230773	29.84%	3.002%
8	7.019	411	414	416	rBV	2347879	2738445	66.40%	6.680%
9	7.419	446	449	451	rBV	2399877	2263445	54.88%	5.522%
10	8.139	510	512	515	rBV	1480757	1538186	37.29%	3.752%
11	9.225	604	607	609	rBV	3921360	4116649	99.81%	10.042%
12	9.613	639	641	643	rBV	767246	642061	15.57%	1.566%
13	9.796	654	657	659	rBV	25787	46905	1.14%	0.114%
14	9.842	659	661	663	rVV	36245	47785	1.16%	0.117%
15	9.899	663	666	668	rVB	2117410	1936664	46.96%	4.724%
16	10.333	703	704	706	rVB	104369	88502	2.15%	0.216%
17	10.562	720	724	727	rBV	27699	54334	1.32%	0.133%
18	10.688	732	735	737	rBV2	2100086	2841143	68.89%	6.931%
19	10.813	744	746	750	rBV	89763	145904	3.54%	0.356%
20	11.259	783	785	786	rBV	115710	103545	2.51%	0.253%
21	11.373	793	795	798	rVB	1422512	1911106	46.34%	4.662%
22	11.682	820	822	824	rBV	104452	83441	2.02%	0.204%
23	11.911	840	842	847	rBV	308515	314089	7.62%	0.766%
24	12.619	900	904	908	rBV2	16900	41537	1.01%	0.101%
25	12.699	908	911	917	rVV	103741	136329	3.31%	0.333%
26	12.791	917	919	923	rVB	65188	62901	1.53%	0.153%
27	12.962	932	934	937	rBV	3176163	4124444	100.00%	10.061%
28	13.454	974	977	982	rBV	255791	641935	15.56%	1.566%
29	13.522	982	983	986	rVB	48137	55887	1.36%	0.136%
30	13.865	1011	1013	1023	rBV	274996	292962	7.10%	0.715%
31	14.014	1023	1026	1028	rBV	1807803	1826981	44.30%	4.457%
32	14.128	1034	1036	1040	rBV3	27517	54367	1.32%	0.133%
33	15.442	1148	1151	1154	rBV	1059719	1279319	31.02%	3.121%
34	15.911	1189	1192	1194	rBV	24032	42867	1.04%	0.105%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EASTWALL-120116

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-BF112916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.957	1194	1196	1201	rVB2	19406	41907	1.02%	0.102%
36	16.402	1230	1235	1242	rBV2	22684	54455	1.32%	0.133%

Sum of corrected areas: 40993134

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
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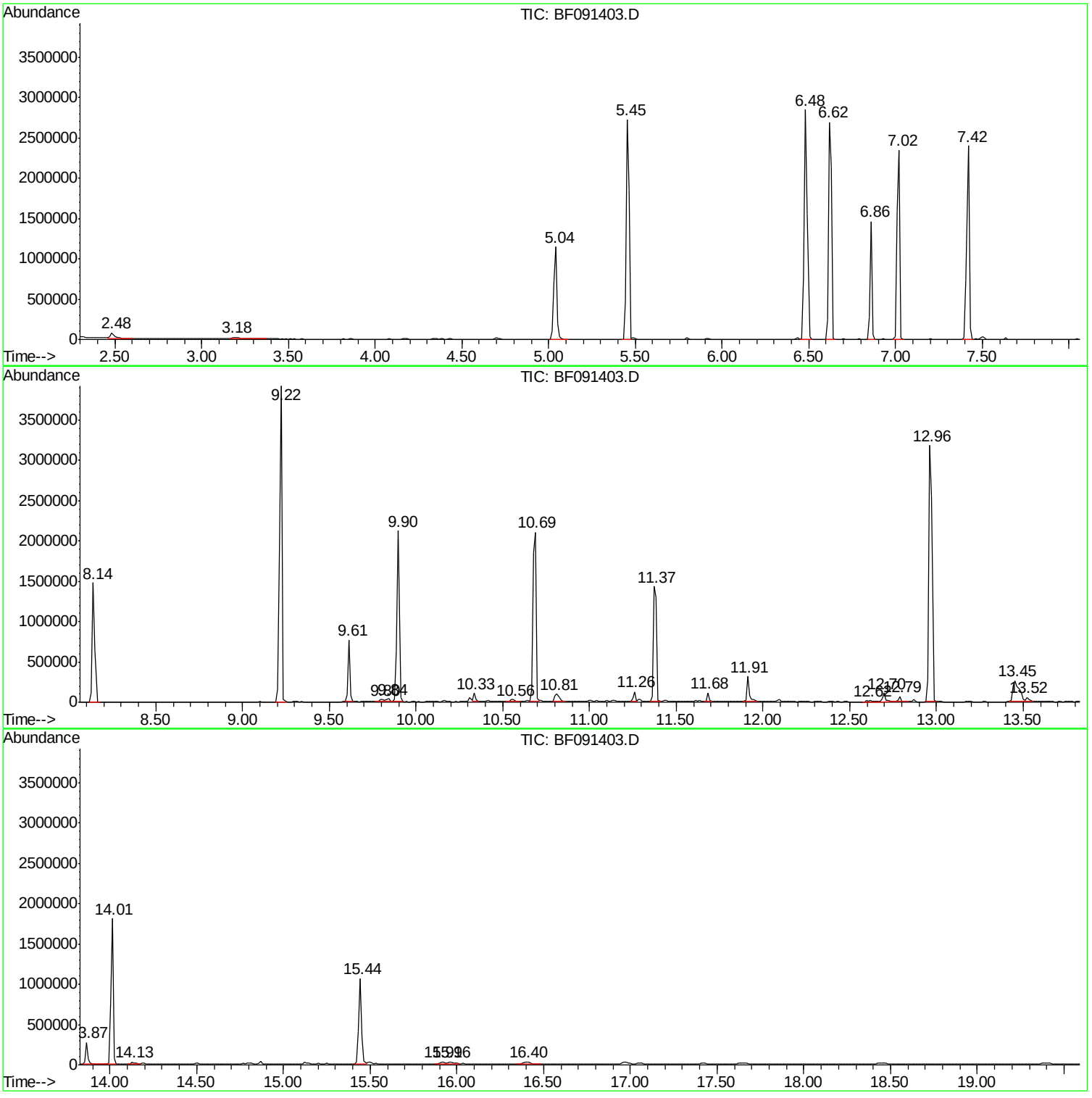
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EASTWALL-120116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

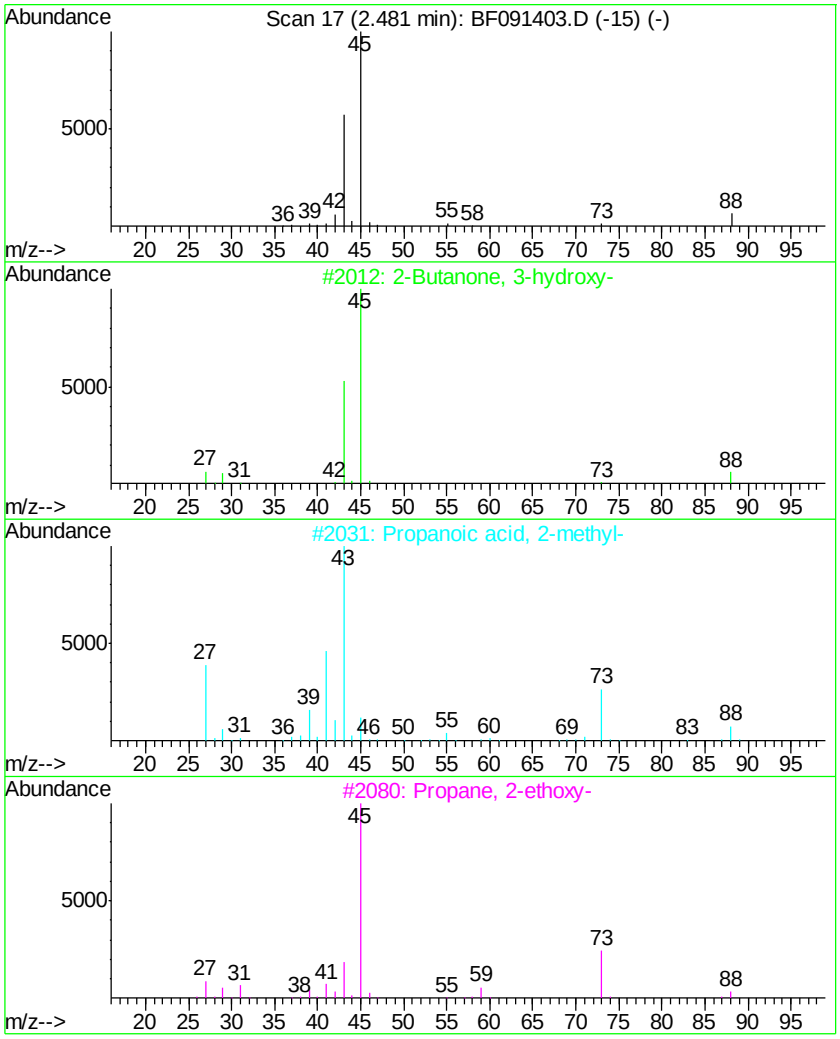
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

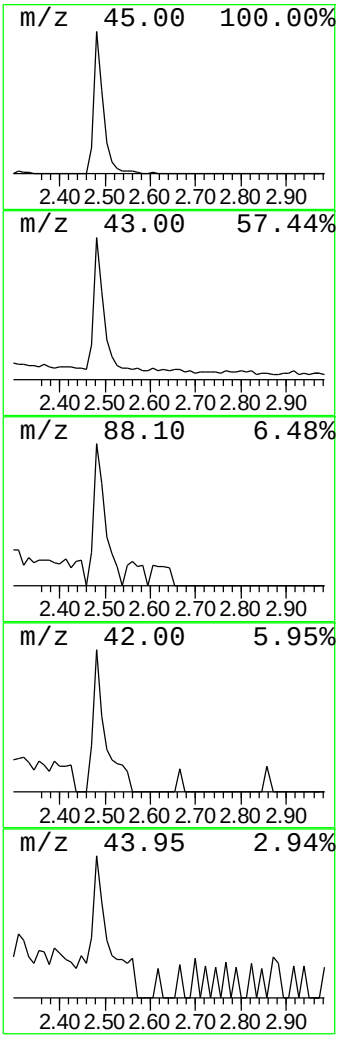
****

Peak Number 1 2-Butanone, 3-hydroxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.48	2.06 ng	126668	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-hydroxy-	88	C4H8O2	000513-86-0	78
2	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	9
3	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
4	Propane, 1-methoxy-2-methyl-	88	C5H12O	000625-44-5	9
5	Ethanol, 2-(vinyloxy)-	88	C4H8O2	000764-48-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EASTWALL-120116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

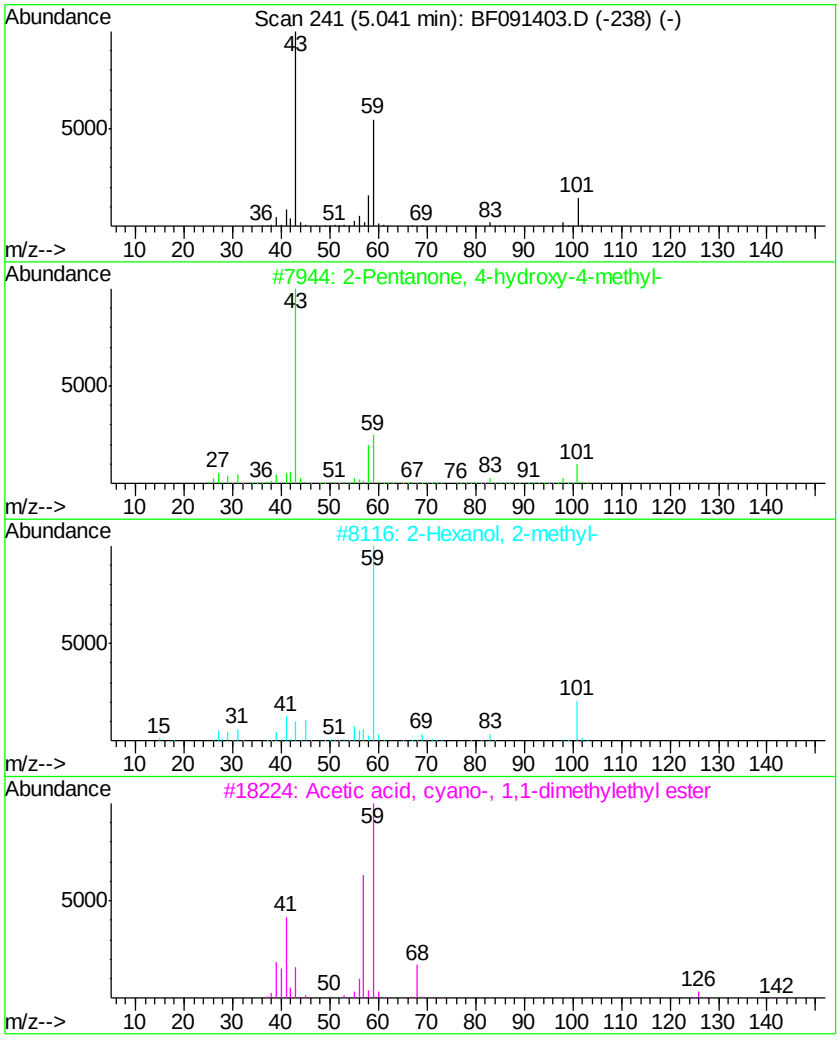
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

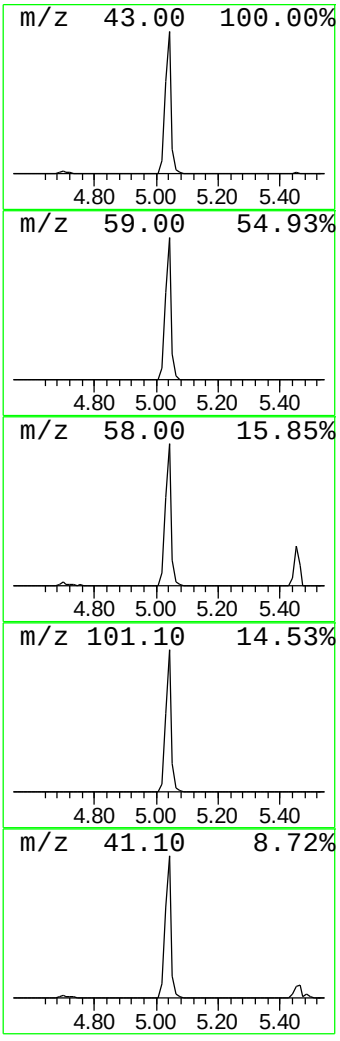
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	24.50 ng	1507800	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
5	1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EASTWALL-120116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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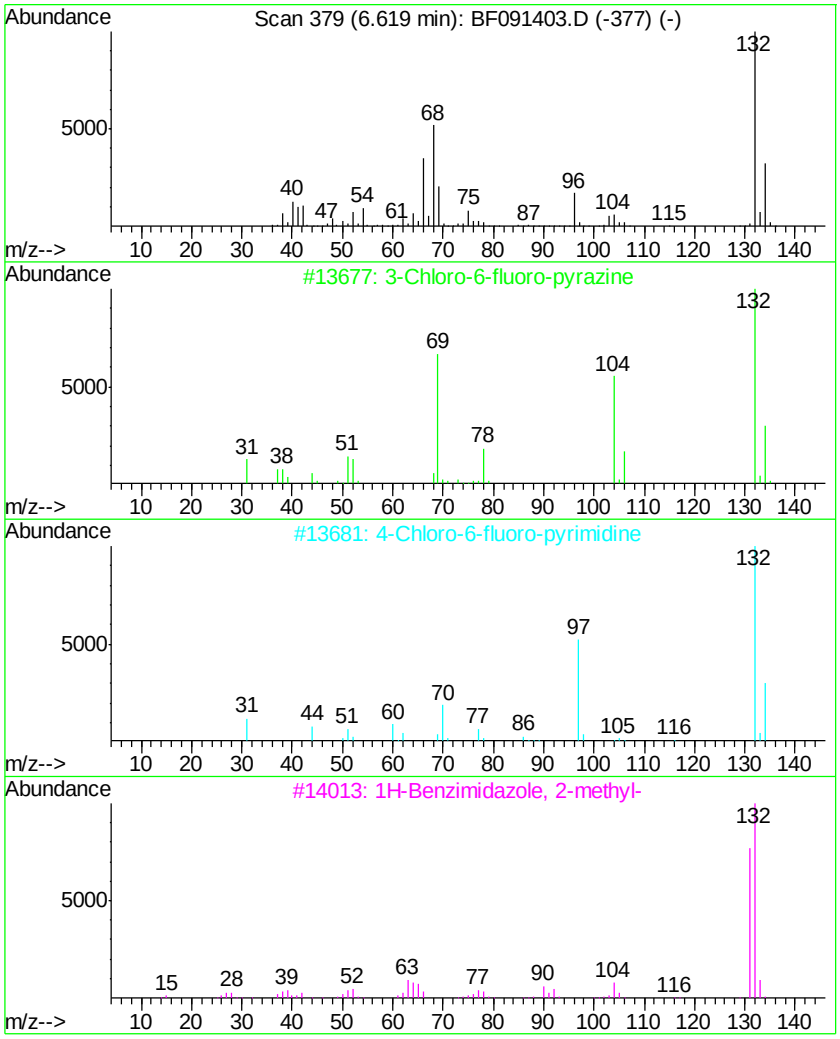
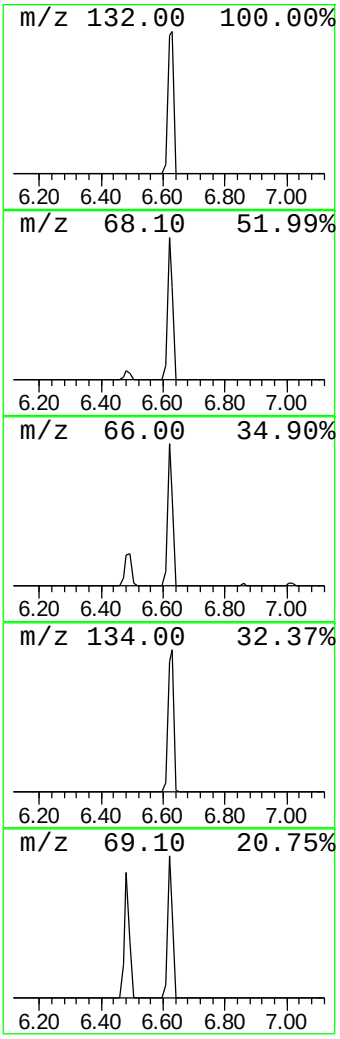
Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	56.56 ng	3480340	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EASTWALL-120116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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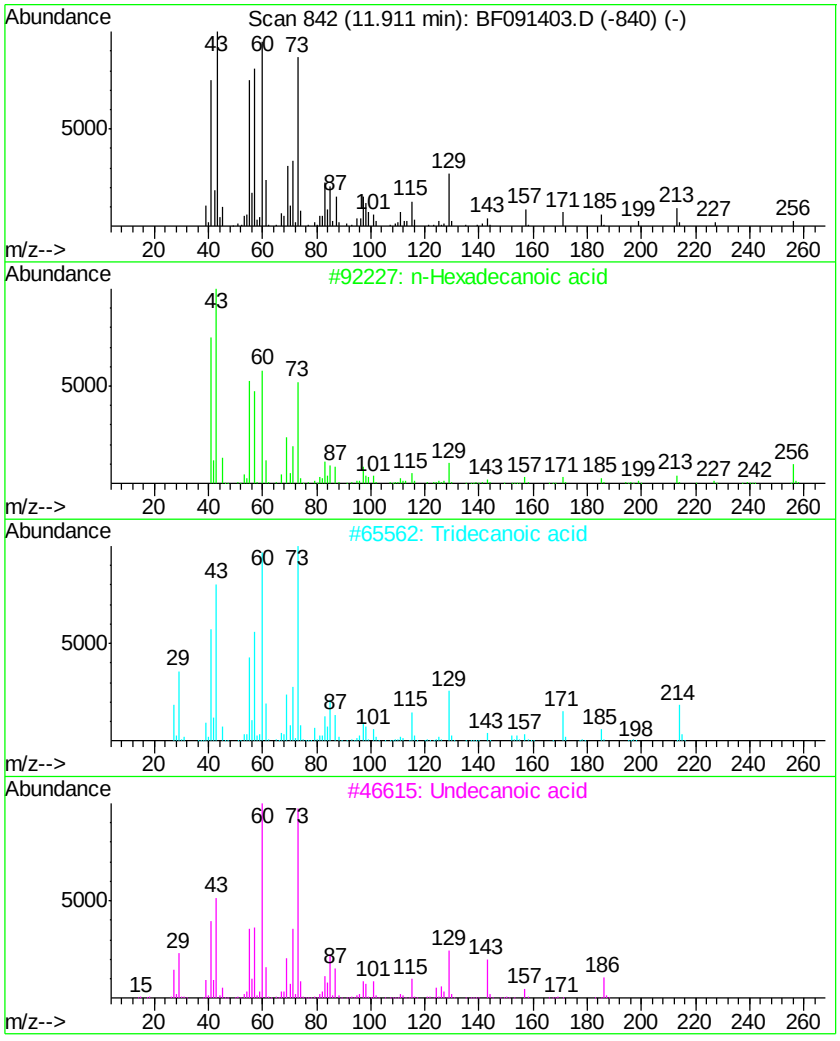
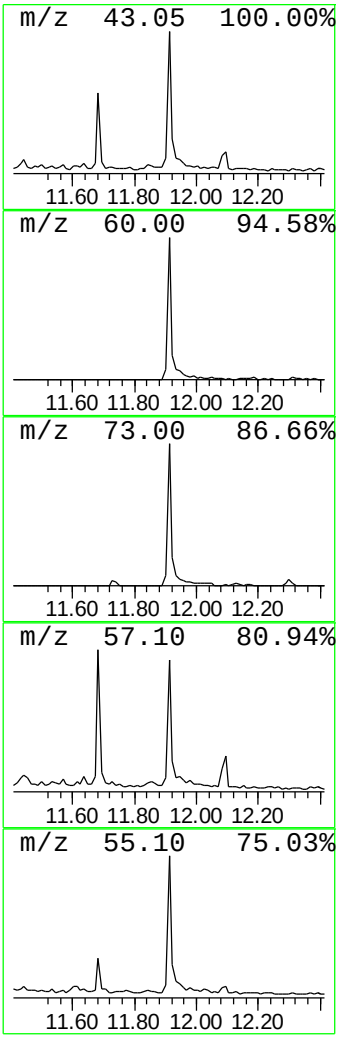
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	3.29 ng	314089	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EASTWALL-120116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

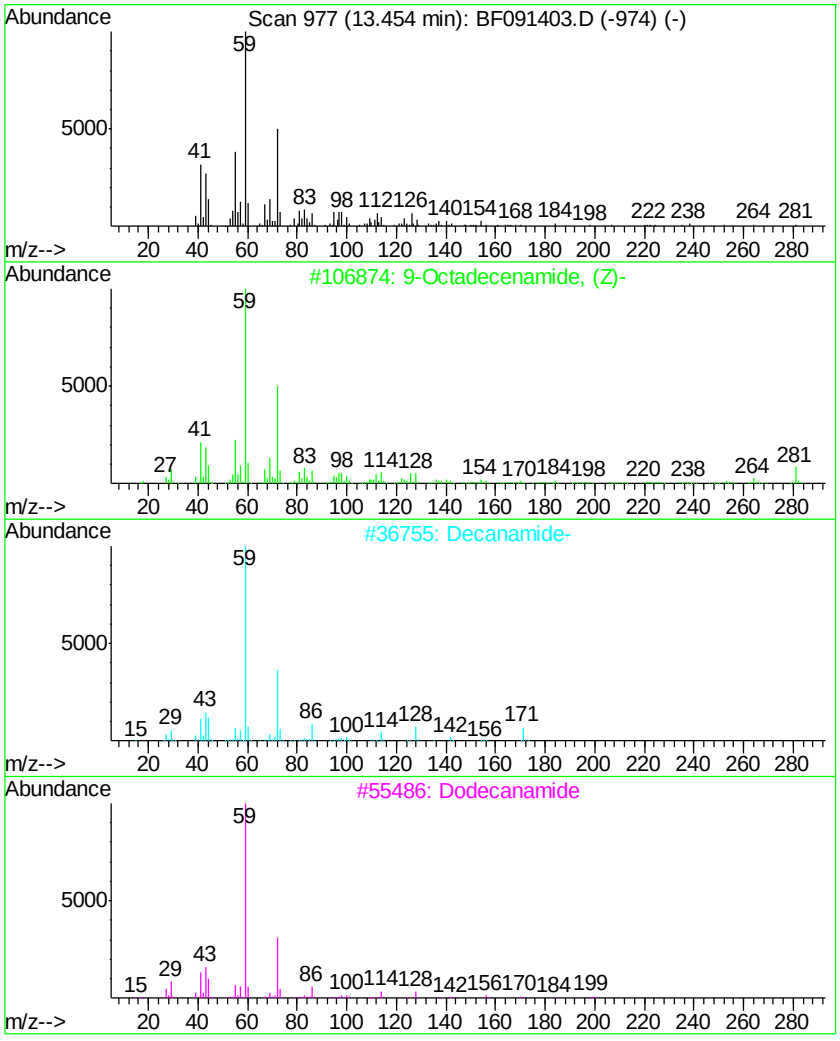
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

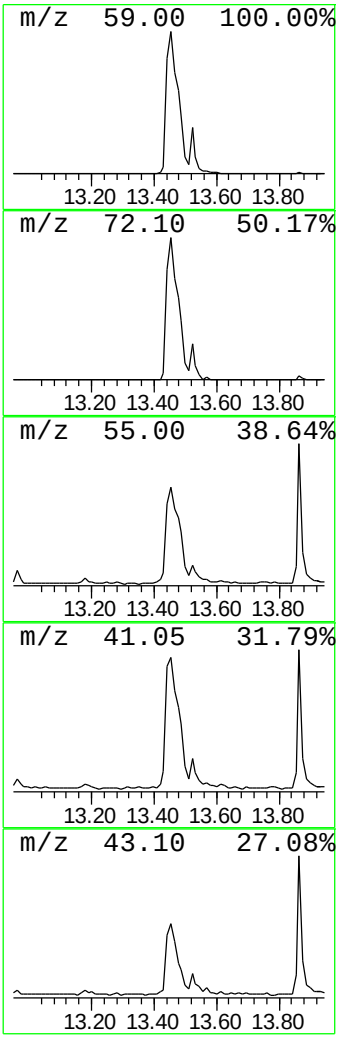
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	7.03 ng	641935	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Decanamide-	171	C10H21NO	002319-29-1	78
3	Dodecanamide	199	C12H25NO	001120-16-7	59
4	Hexadecanamide	255	C16H33NO	000629-54-9	59
5	Nonanamide	157	C9H19NO	001120-07-6	53





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EASTWALL-120116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

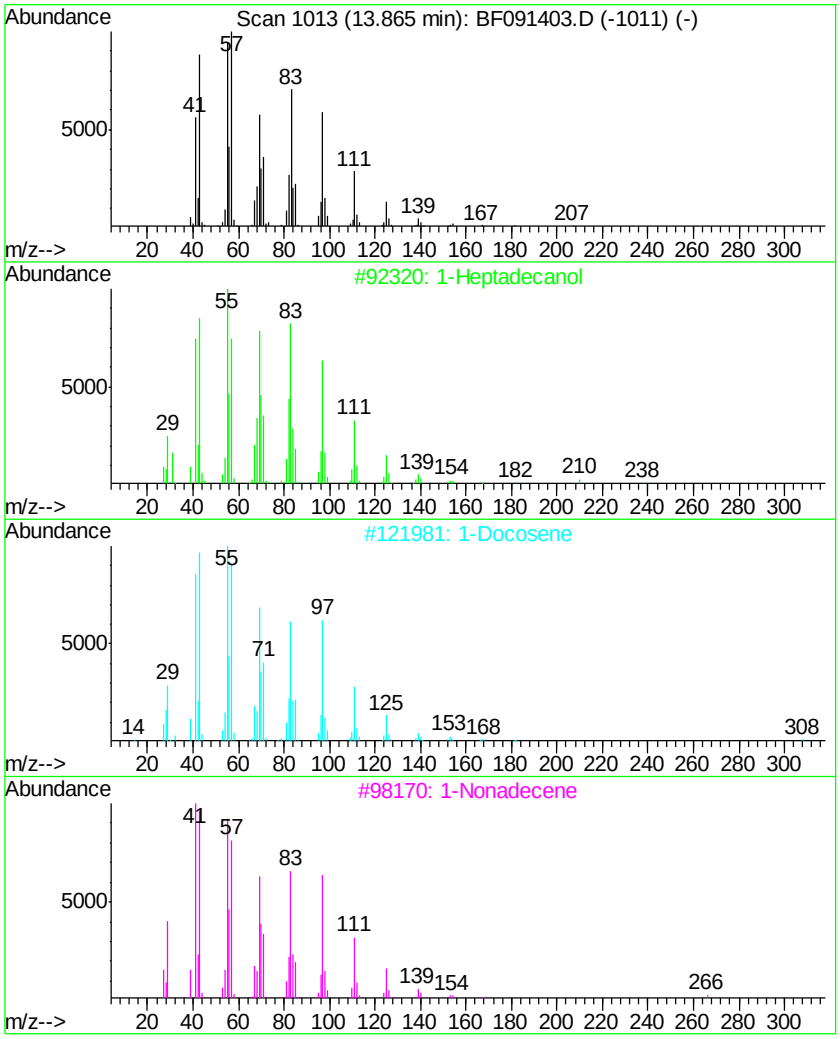
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

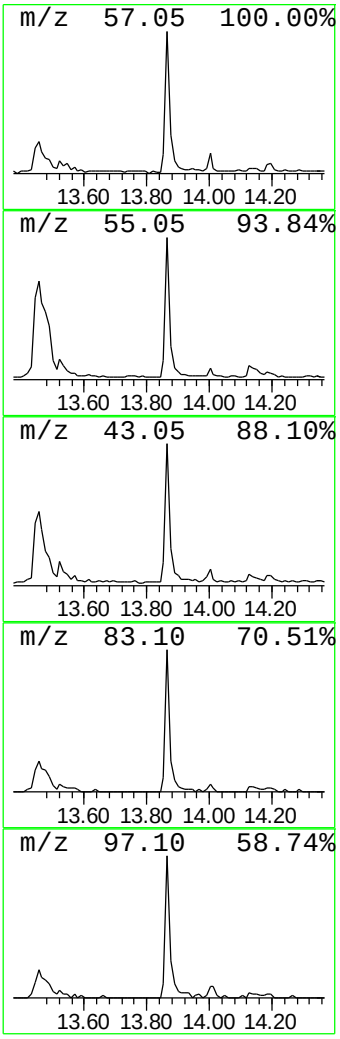
****

Peak Number 7 1-Heptadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.21 ng	292962	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecanol	256	C17H36O	001454-85-9	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120216\
Data File : BF091403.D
Acq On : 2 Dec 2016 21:43
Operator : UM/SJ
Sample : H5829-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EASTWALL-120116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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
2-Butanone, 3-hyd...	2.48	2.1	ng	126668	1	6.86	1230770	20.0
2-Pentanone, 4-hy...	5.04	24.5	ng	1507800	1	6.86	1230770	20.0
unknown6.62	6.62	56.6	ng	3480340	1	6.86	1230770	20.0
n-Hexadecanoic acid	11.91	3.3	ng	314089	4	11.38	1911110	20.0
9-Octadecenamide,...	13.45	7.0	ng	641935	5	14.01	1826980	20.0
1-Heptadecanol	13.87	3.2	ng	292962	5	14.01	1826980	20.0