LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096841.D
Acq On : 18 Jul 2017 12:07
Operator : SJ/JU
Sample : I4199-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3574-PA4

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-BF071317.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	4.763	468	472	481	rVB	123758	153213	4.47%	0.639%
2	5.204	543	547	554	rBV	1616863	1488013	43.43%	6.206%
3	6.245	720	724	733	rVB	1027028	927258	27.06%	3.868%
4	6.369	740	745	748	rBV	2691631	2567535	74.93%	10.709%
5	6.598	780	784	787	rBV	738837	671011	19.58%	2.799%
6	6.757	806	811	814	rBV	2340517	2312415	67.48%	9.645%
7	7.163	874	880	883	rBV	2093739	2269513	66.23%	9.466%
8	7.881	998	1002	1005	rBV	1055286	981500	28.64%	4.094%
9	8.157	1044	1049	1052	rBV	957905	844830	24.65%	3.524%
10	8.251	1060	1065	1070	rBV2	34479	57323	1.67%	0.239%
11	8.963	1177	1186	1189	rVB	3039442	3426616	100.00%	14.292%
12	9.392	1254	1259	1263	rBV7	39783	51745	1.51%	0.216%
13	9.627	1294	1299	1303	rBV2	1257879	1110496	32.41%	4.632%
14	10.251	1402	1405	1408	rBV	91339	90008	2.63%	0.375%
15	10.416	1428	1433	1436	rBV	1858510	1896258	55.34%	7.909%
16	10.527	1448	1452	1456	rVB	263426	266643	7.78%	1.112%
17	10.827	1500	1503	1506	rVB	60356	56709	1.65%	0.237%
18	11.104	1546	1550	1553	rBV	950701	806728	23.54%	3.365%
19	11.504	1615	1618	1621	rBV3	51990	45081	1.32%	0.188%
20	11.657	1641	1644	1650	rVB2	131732	153537	4.48%	0.640%
21	11.827	1670	1673	1676	rBV	76847	80235	2.34%	0.335%
22	12.439	1774	1777	1784	rBV	206320	209817	6.12%	0.875%
23	12.692	1815	1820	1823	rBV	2318204	2379368	69.44%	9.924%
24	13.727	1993	1996	2000	rVB	671570	601305	17.55%	2.508%
25	15.104	2226	2230	2234	rVB	497187	528324	15.42%	2.204%

Sum of corrected areas: 23975481

LSC Report - Integrated Chromatogram

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Misc :
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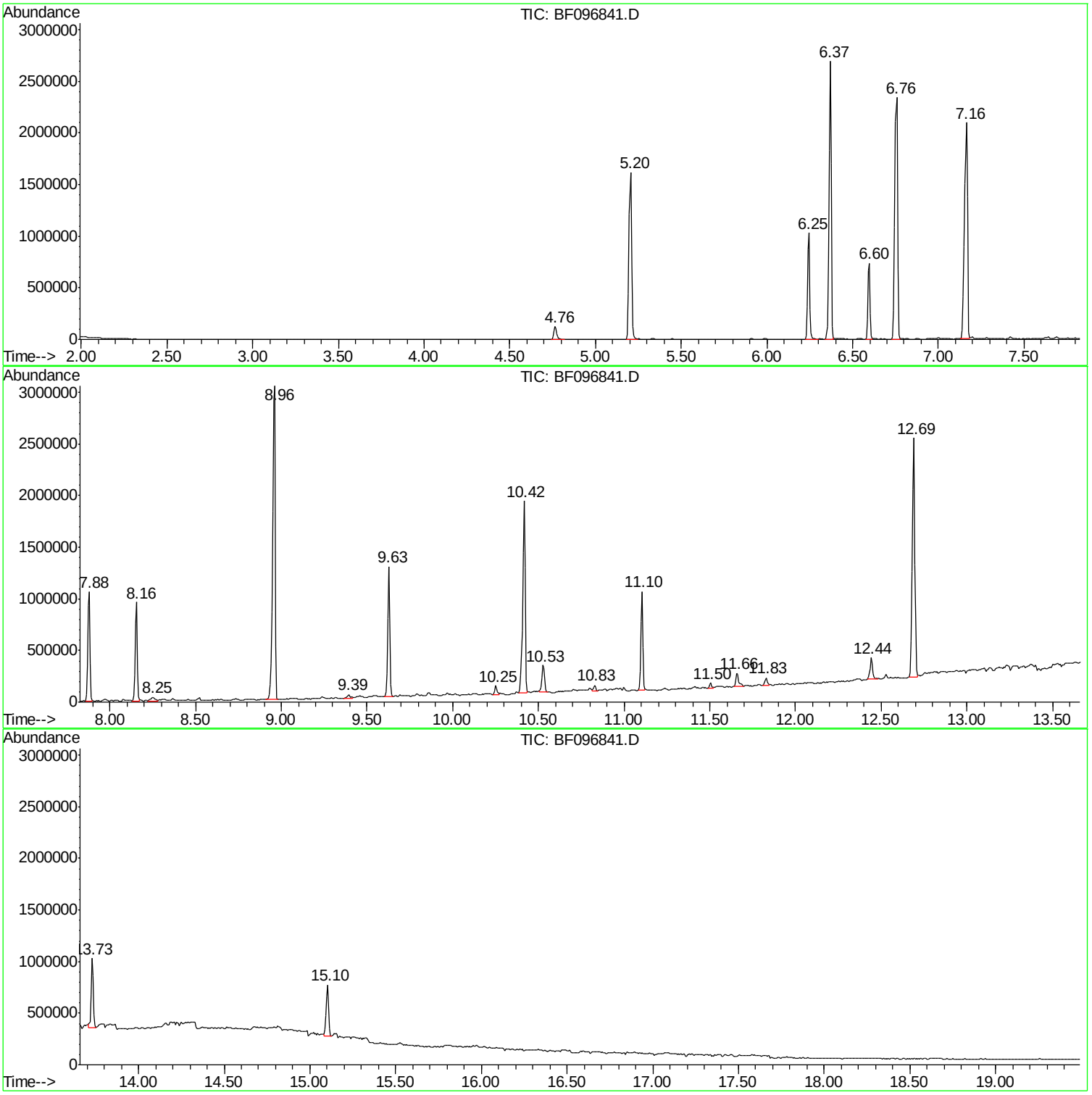
Instrument : BNA_F
ClientSampleId : 3574-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096841.D
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Operator : SJ/JU
Sample : I4199-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3574-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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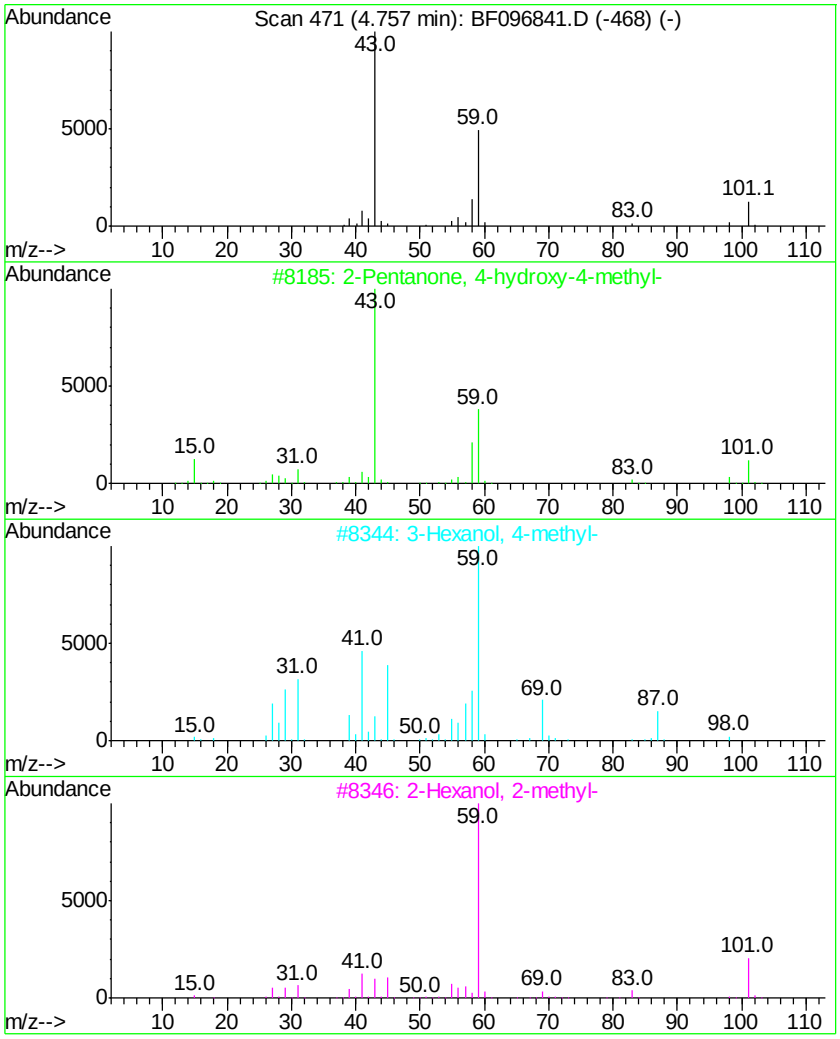
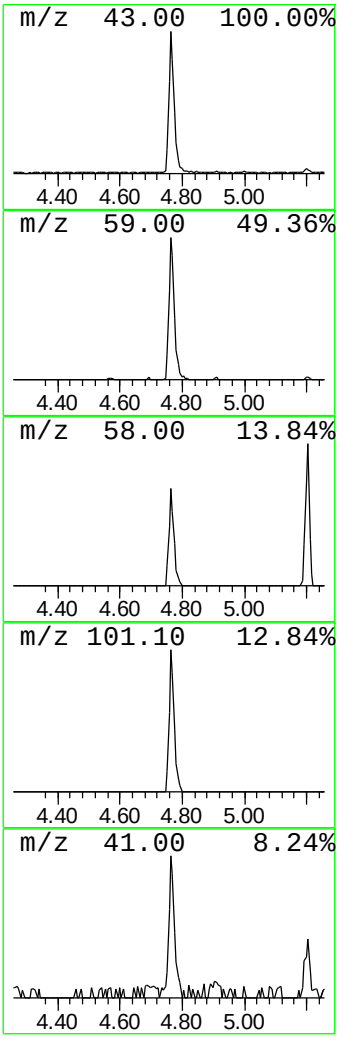
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	4.57 ng	153213	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





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Data File : BF096841.D
Acq On : 18 Jul 2017 12:07
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Sample : I4199-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3574-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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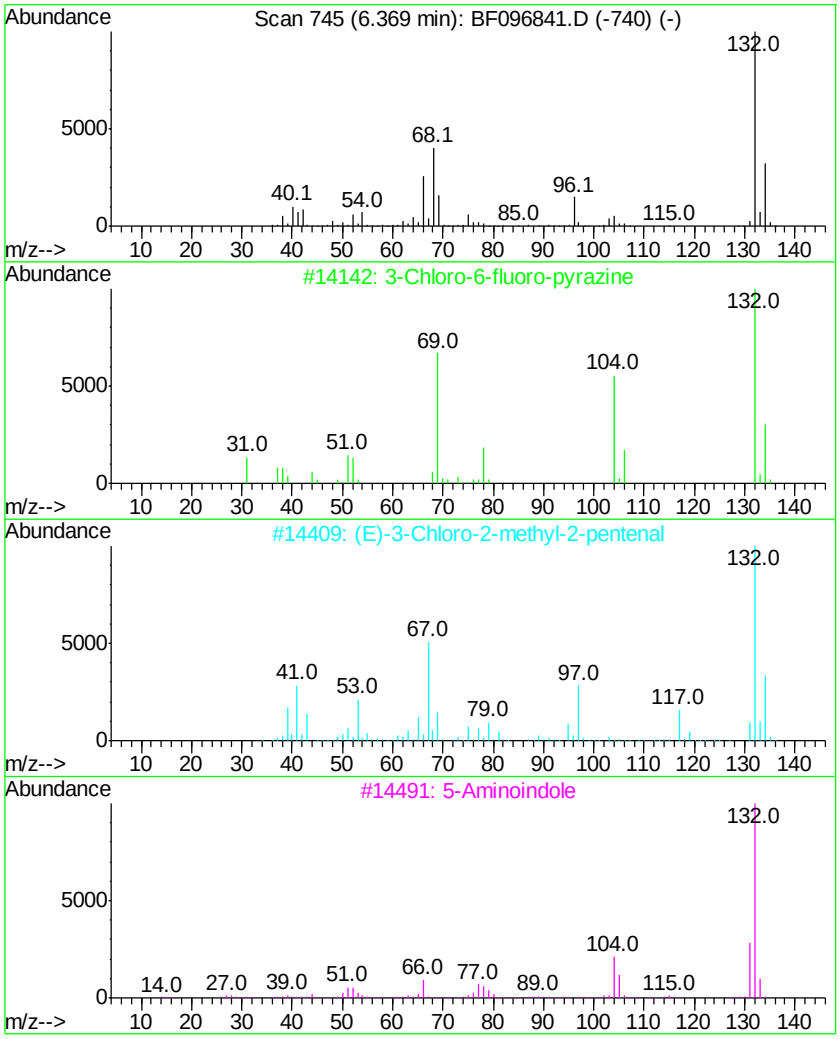
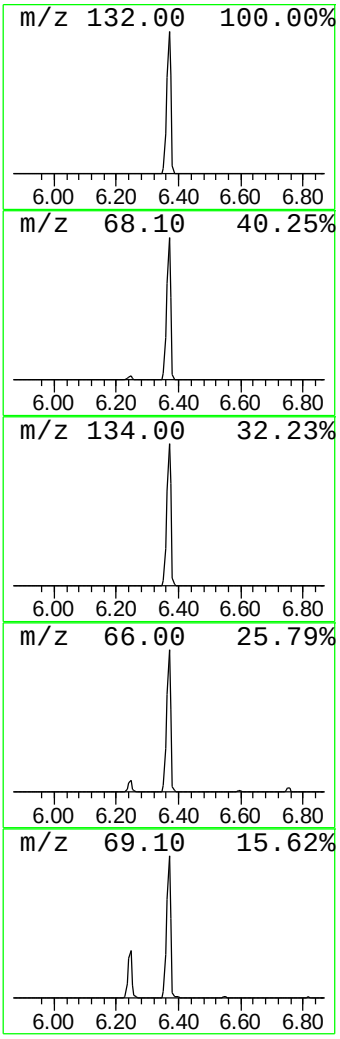
Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	76.53 ng	2567540	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096841.D
Acq On : 18 Jul 2017 12:07
Operator : SJ/JU
Sample : I4199-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3574-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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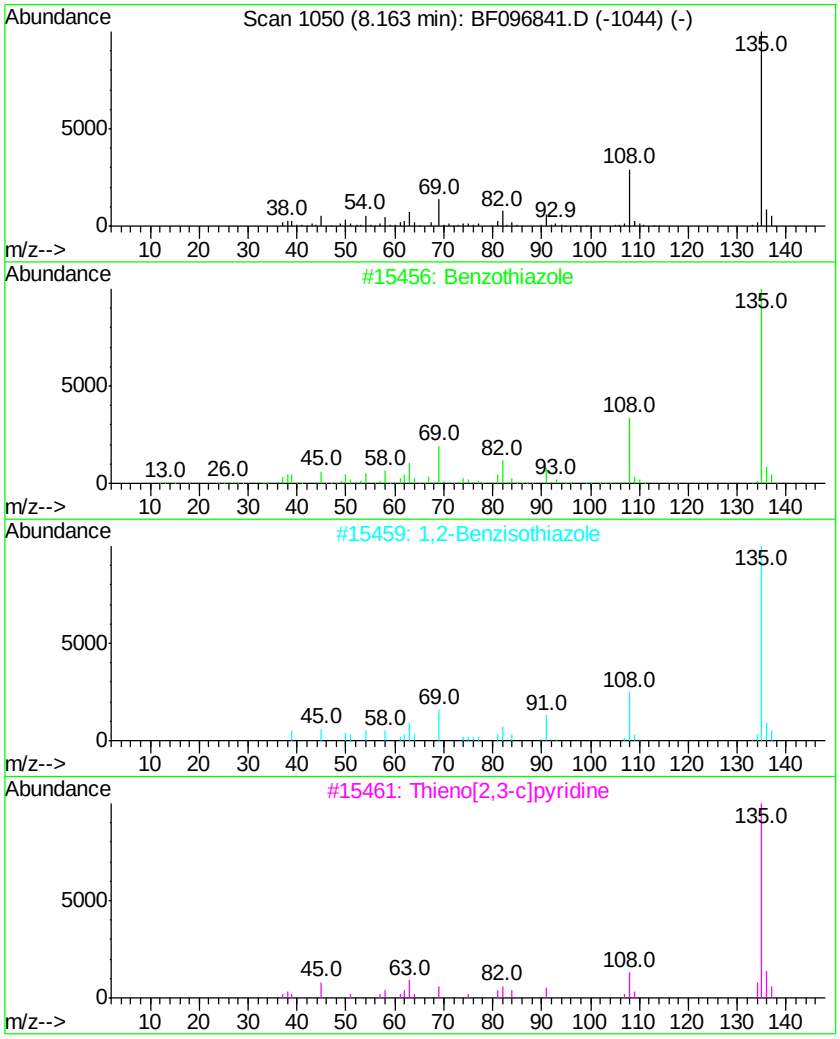
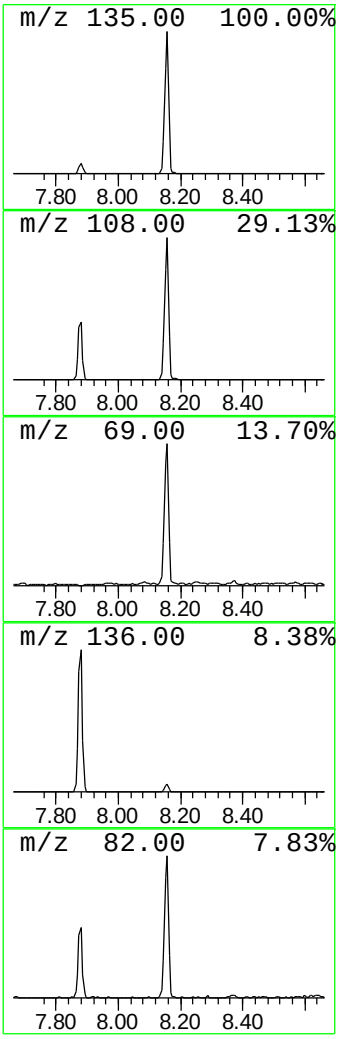
Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	17.22 ng	844830	Naphthalene-d8	7.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	97
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	80
4	2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	64
5	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096841.D
Acq On : 18 Jul 2017 12:07
Operator : SJ/JU
Sample : I4199-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3574-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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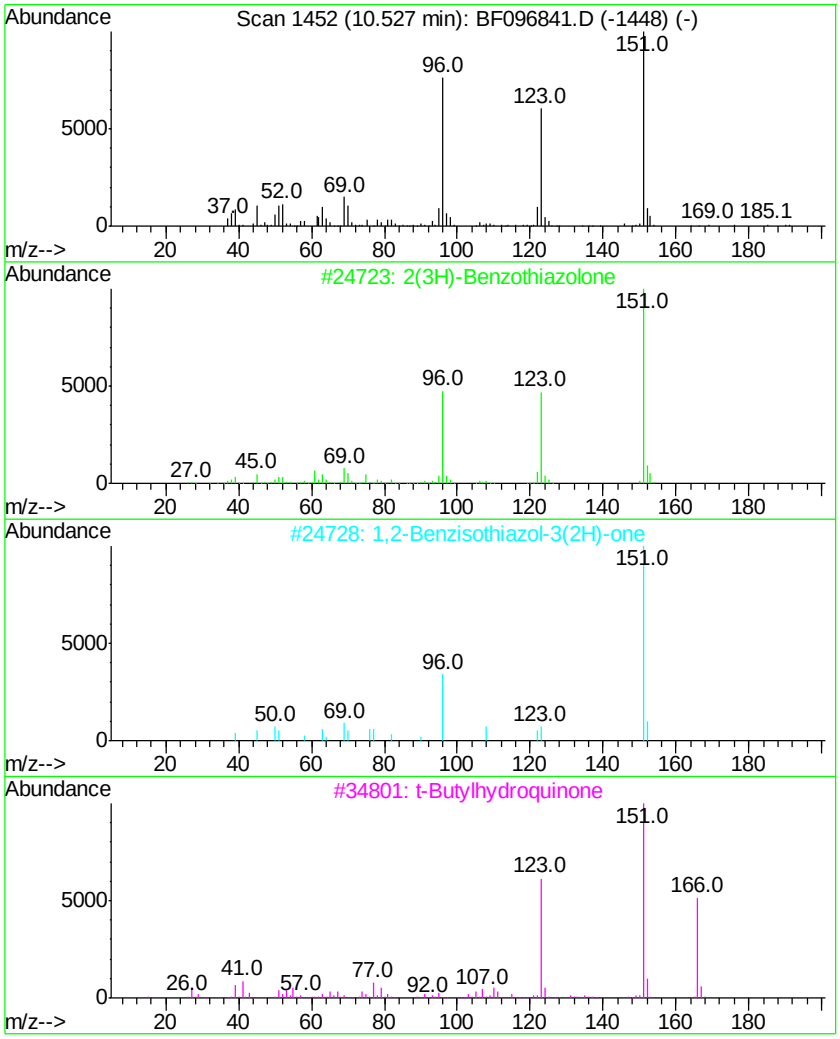
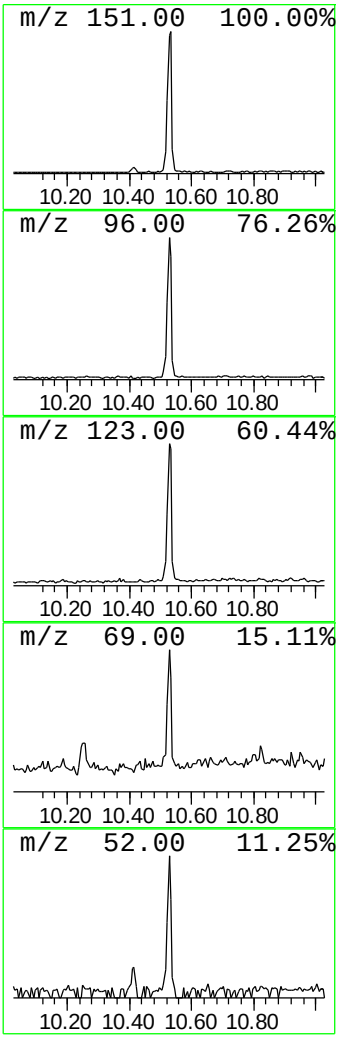
Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	6.61 ng	266643	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
3	t-Butylhydroquinone	166	C10H14O2	001948-33-0	43
4	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	38
5	2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	35





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Data File : BF096841.D
Acq On : 18 Jul 2017 12:07
Operator : SJ/JU
Sample : I4199-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3574-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

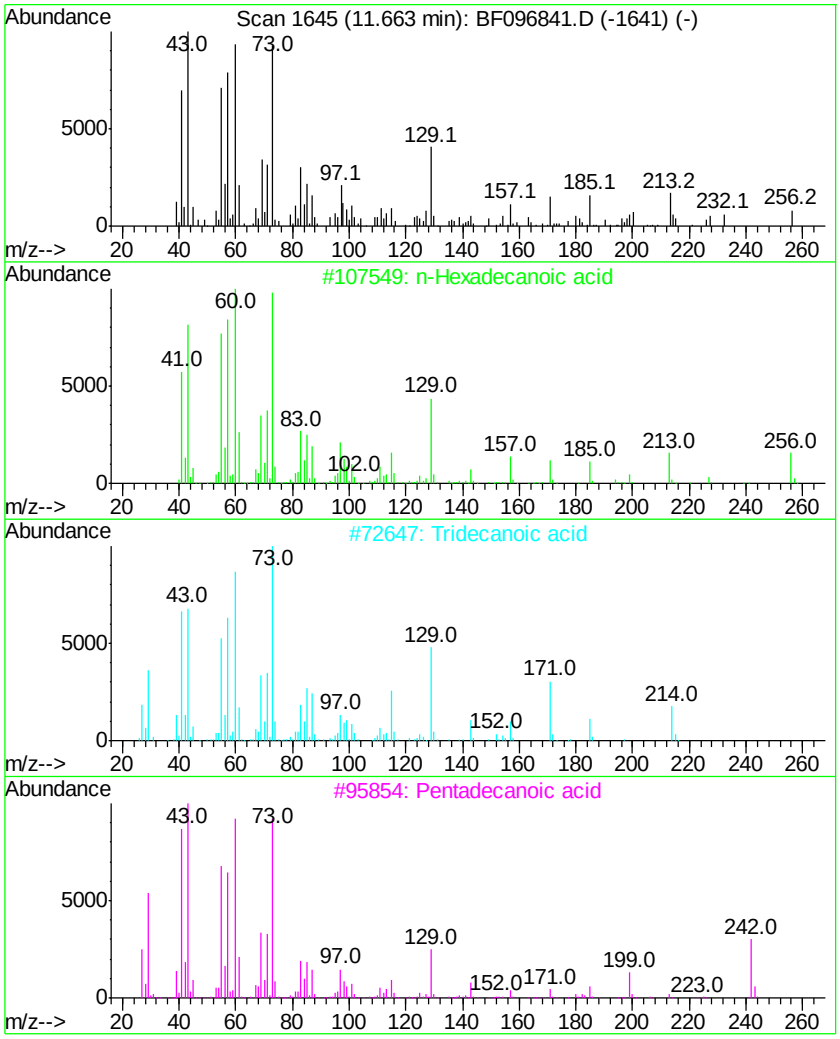
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

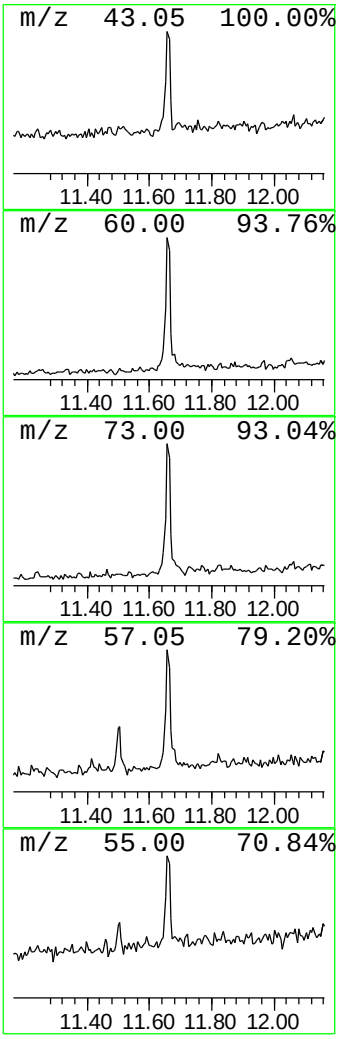
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	3.81 ng	153537	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
Data File : BF096841.D
Acq On : 18 Jul 2017 12:07
Operator : SJ/JU
Sample : I4199-12
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3574-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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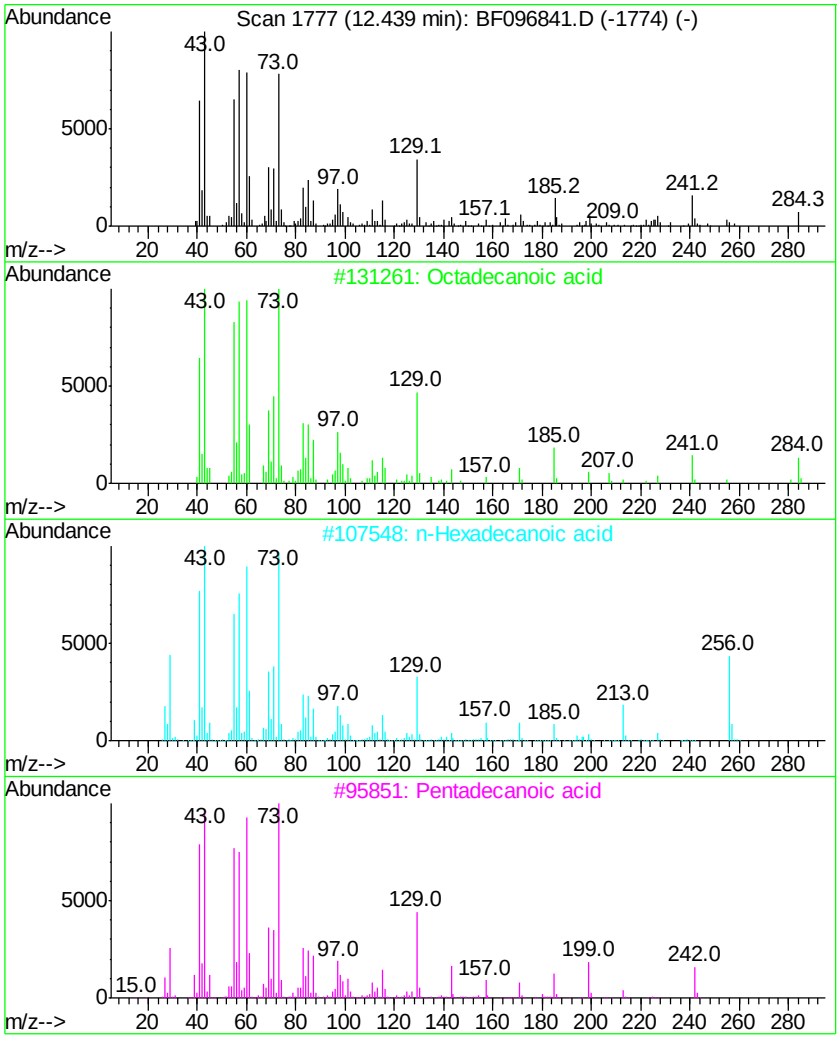
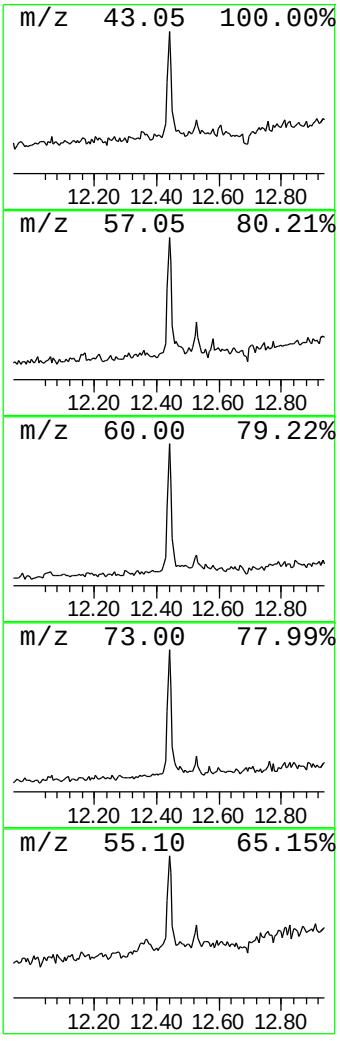
Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	6.98 ng	209817	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Dodecanoic acid	200	C12H24O2	000143-07-7	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	4.76	4.6	ng	153213	1	6.60	671011	20.0
unknown6.37	6.37	76.5	ng	2567540	1	6.60	671011	20.0
Benzothiazole	8.16	17.2	ng	844830	2	7.88	981500	20.0
2(3H)-Benzothiazo...	10.53	6.6	ng	266643	4	11.10	806728	20.0
n-Hexadecanoic acid	11.66	3.8	ng	153537	4	11.10	806728	20.0
Octadecanoic acid	12.44	7.0	ng	209817	5	13.73	601305	20.0