LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

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-BF072016.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	1.712	9	11	49	rVB	423750	913704	7.18%	2.827%
2	5.153	310	312	332	rBV9	370661	617979	4.86%	1.912%
3	6.250	404	408	414	rBV2	873389	1392295	10.94%	4.307%
4	6.341	414	416	431	rVB	771050	1202669	9.45%	3.721%
5	6.582	434	437	439	rBV	221870	261574	2.06%	0.809%
6	6.662	442	444	447	rBV	732442	790054	6.21%	2.444%
7	6.730	448	450	453	rBV	920440	996475	7.83%	3.083%
8	7.153	484	487	495	rBV	837067	1049270	8.25%	3.246%
9	7.347	495	504	510	rVB	133090	392236	3.08%	1.213%
10	7.793	541	543	547	rBV2	88041	128911	1.01%	0.399%
11	7.862	547	549	560	rVB	392779	428065	3.36%	1.324%
12	8.147	572	574	581	rBV	1058280	1147109	9.02%	3.549%
13	8.947	641	644	646	rBV	1757622	1913667	15.04%	5.920%
14	9.610	699	702	704	rBV	447771	458822	3.61%	1.419%
15	9.862	721	724	730	rBV	164005	244744	1.92%	0.757%
16	10.399	768	771	780	rBV	916771	1058295	8.32%	3.274%
17	10.548	780	784	789	rBV	402763	713579	5.61%	2.208%
18	11.085	828	831	835	rBV	427680	464295	3.65%	1.436%
19	11.828	894	896	901	rVV	286925	620972	4.88%	1.921%
20	11.908	901	903	914	rVV	548886	1285522	10.10%	3.977%
21	12.159	914	925	926	rVV	3504557	12722880	100.00%	39.359%
22	12.182	926	927	939	rVB	397497	719112	5.65%	2.225%
23	12.674	967	970	972	rBV	1621492	1769791	13.91%	5.475%
24	12.936	986	993	1001	rVV3	152769	406887	3.20%	1.259%
25	13.702	1058	1060	1068	rVB	331883	372201	2.93%	1.151%
26	15.051	1175	1178	1187	rVB	157800	254011	2.00%	0.786%

Sum of corrected areas: 32325119

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Operator : UM/SJ
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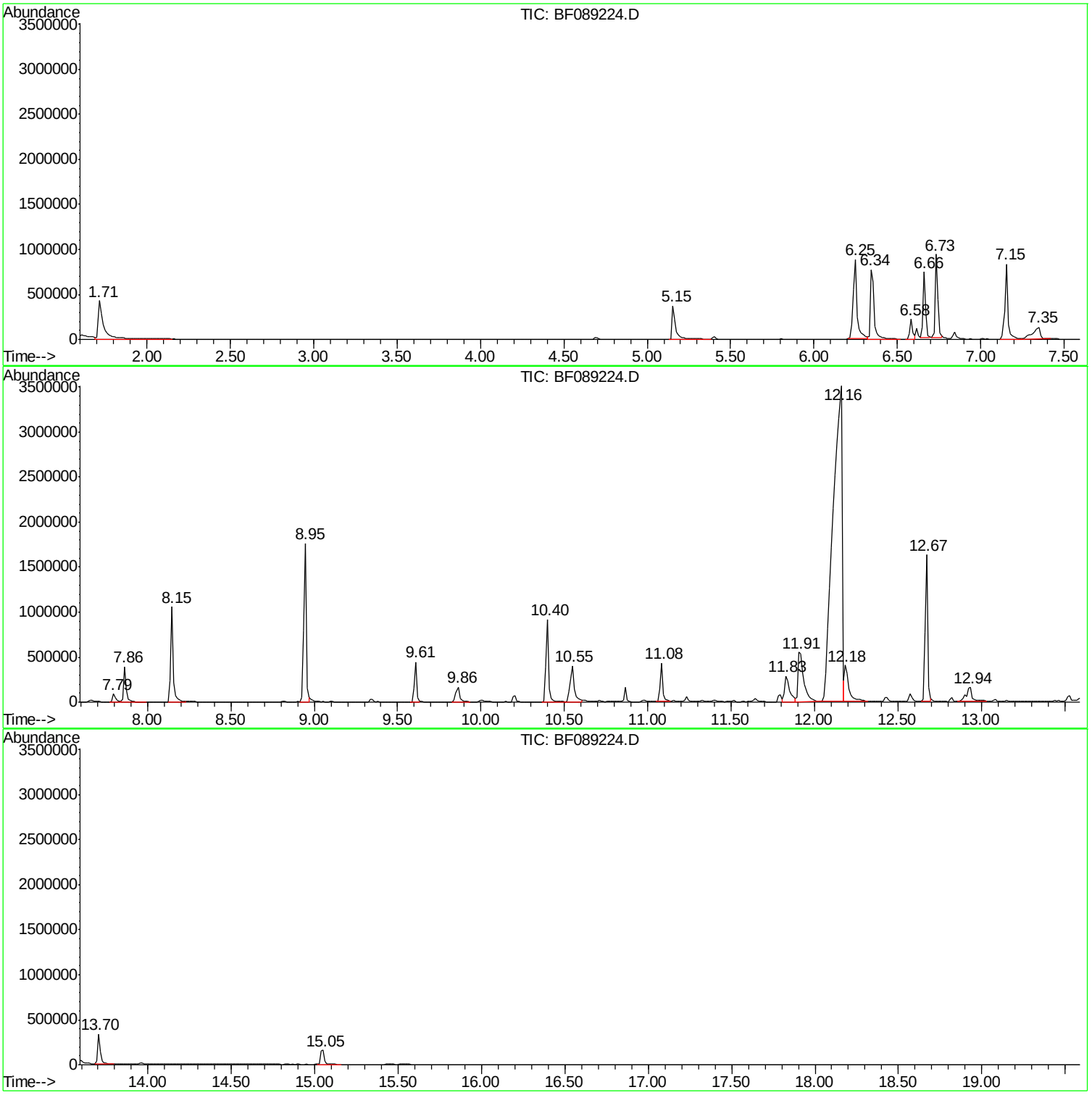
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

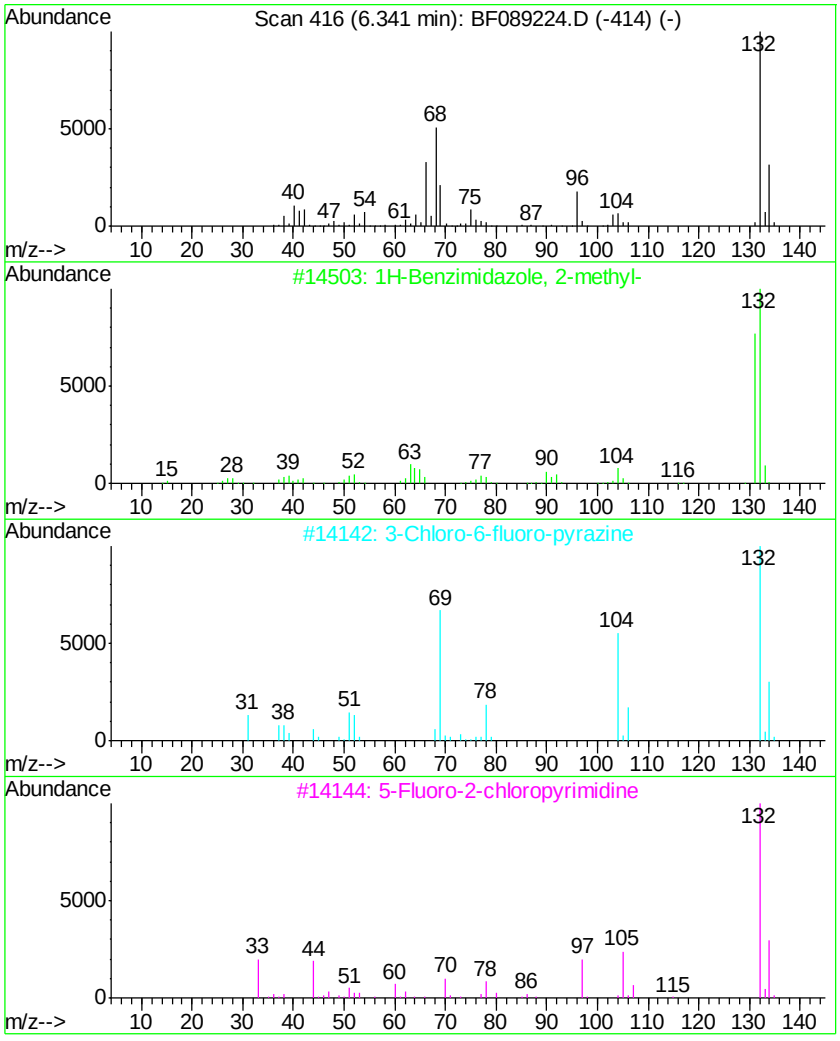
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

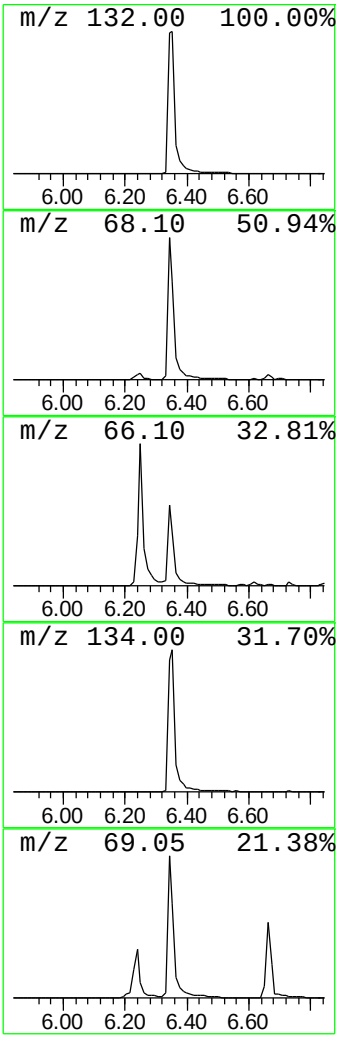
****

Peak Number 2 unknown6.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	91.96 ng	1202670	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

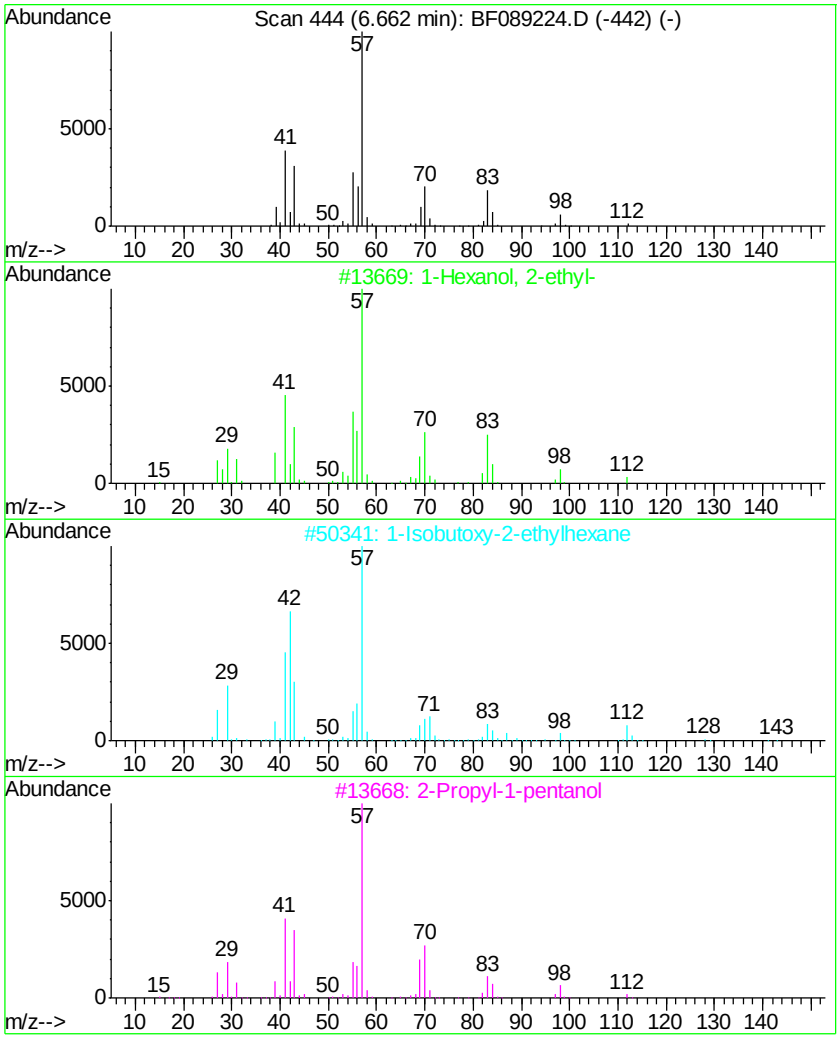
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

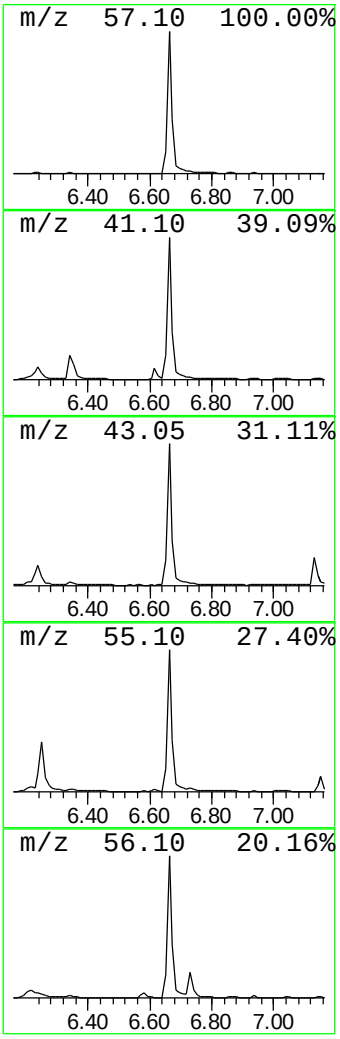
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	60.41 ng	790054	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

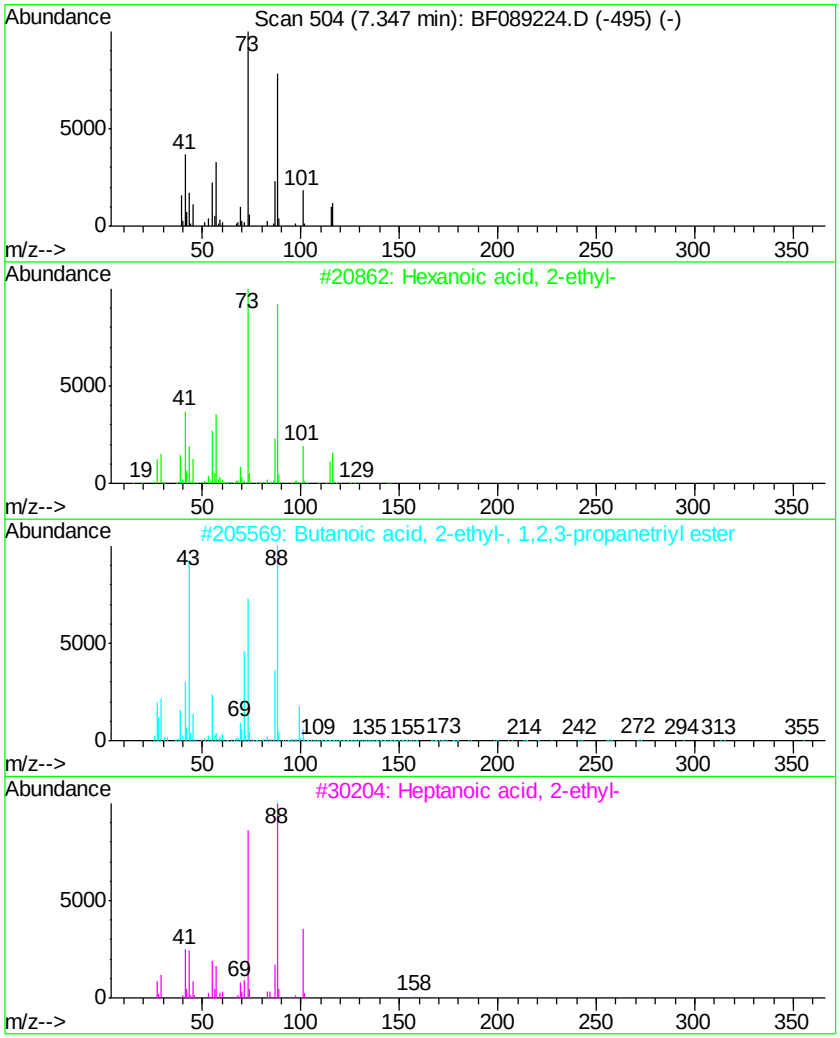
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

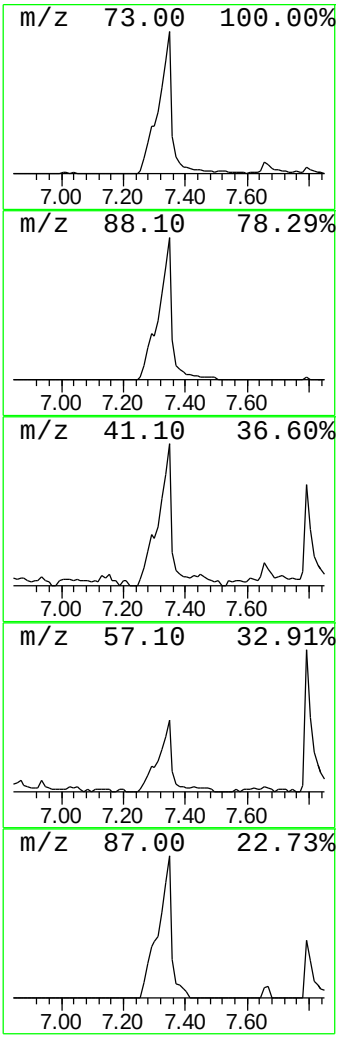
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.35	18.33 ng	392236	Naphthalene-d8	7.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	40
4	Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	40
5	1,4-Dioxane	88	C4H8O2	000123-91-1	37





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
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Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

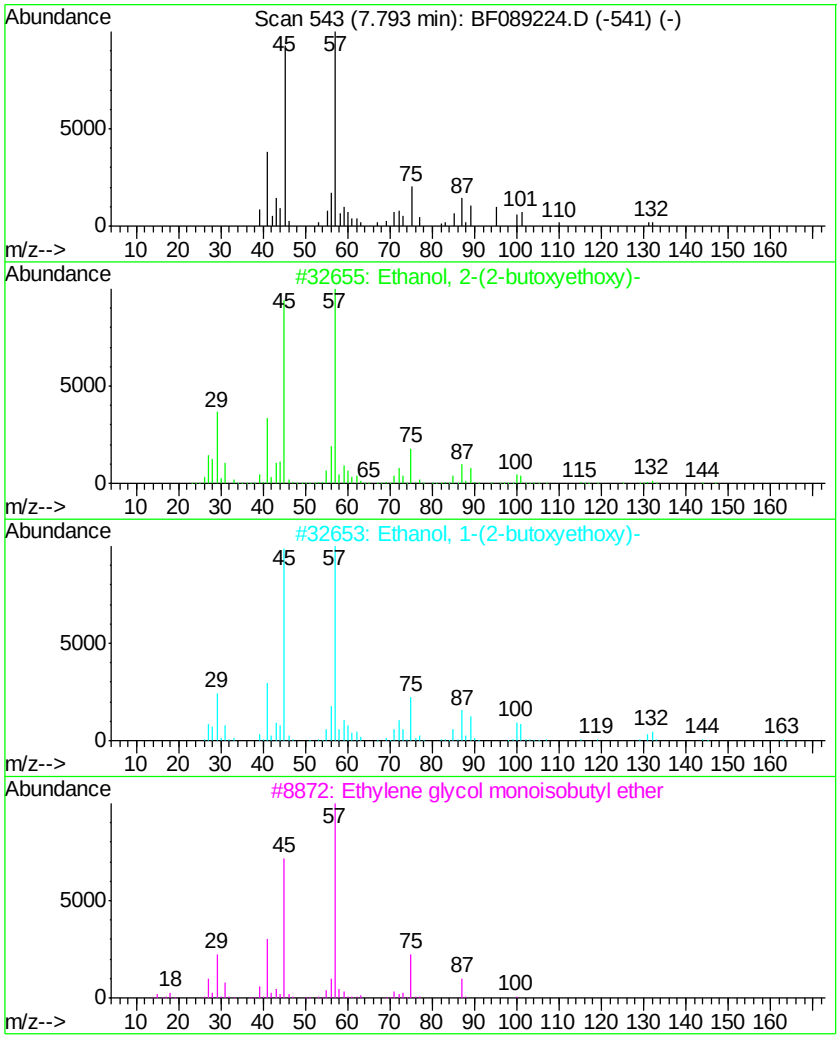
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

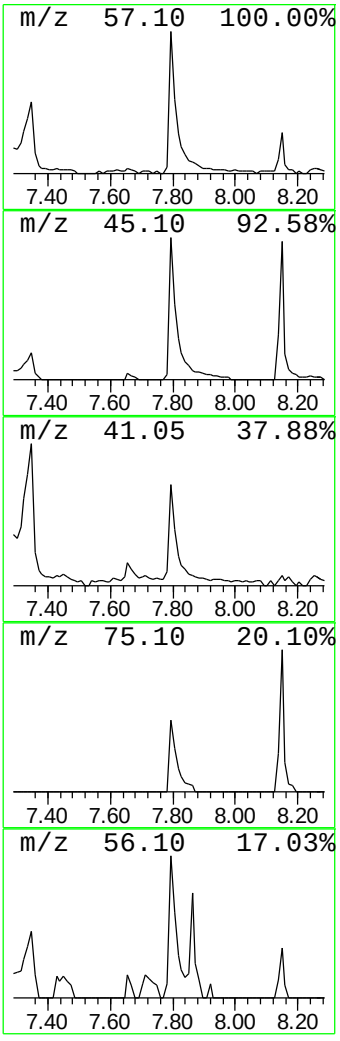
****

Peak Number 6 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	6.02 ng	128911	Naphthalene-d8	7.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	45
5	2-Propanol, 1-(2-methylpropoxy)-	132	C7H16O2	023436-19-3	40





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

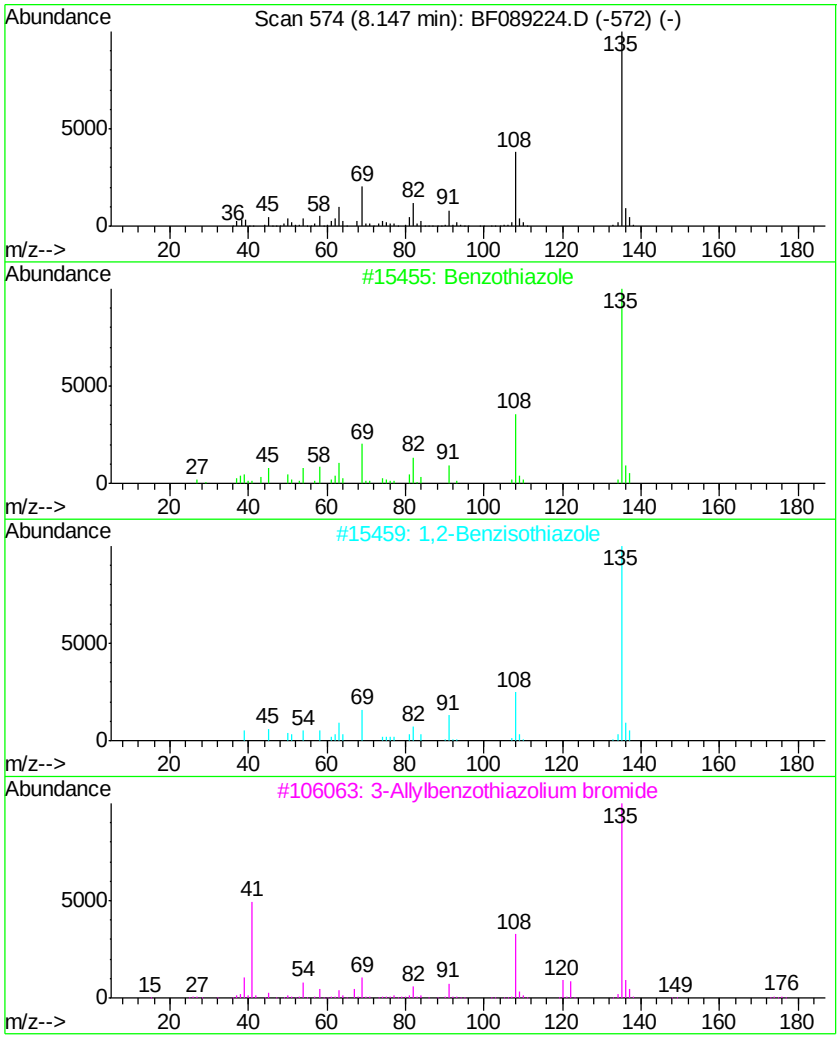
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

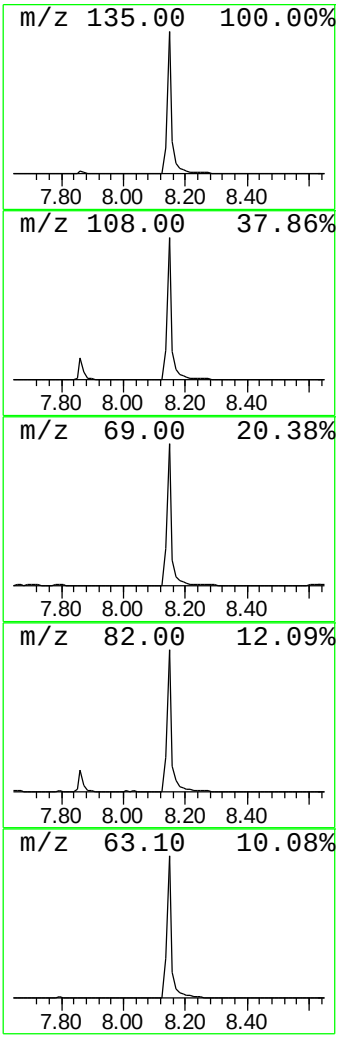
****

Peak Number 7 Benzothiazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.15	53.60 ng	1147110	Naphthalene-d8	7.86

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	83
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	78
4	2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	72
5	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

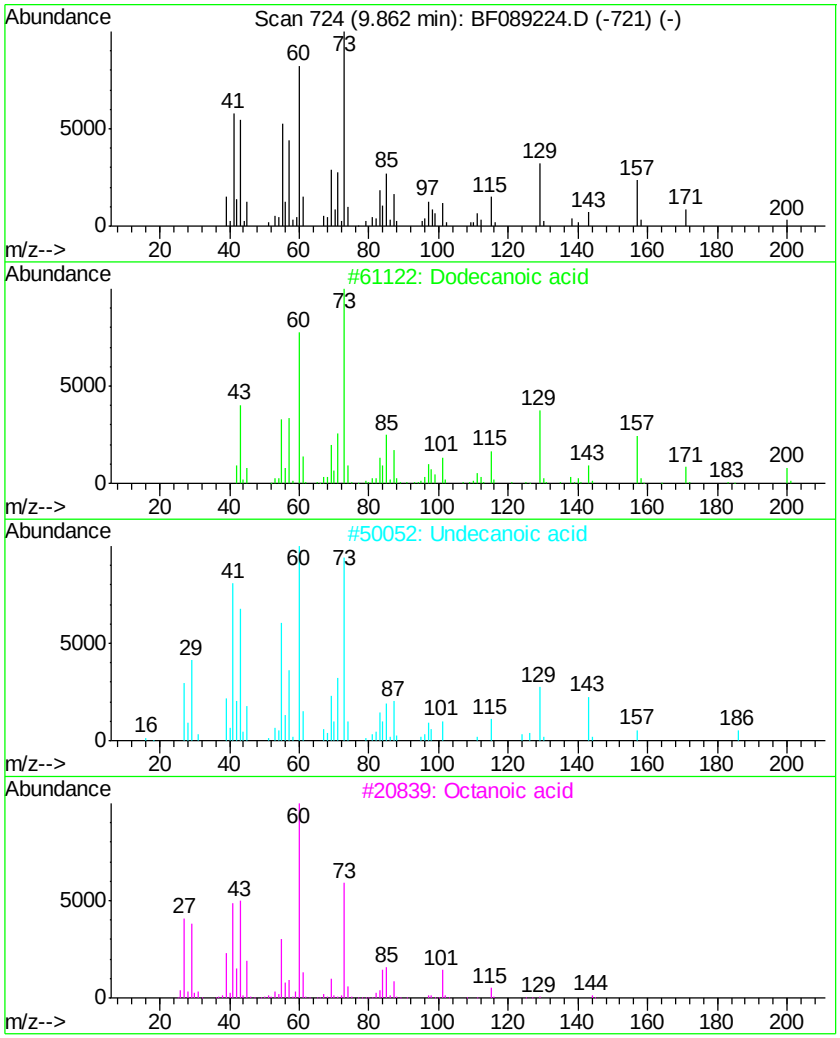
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

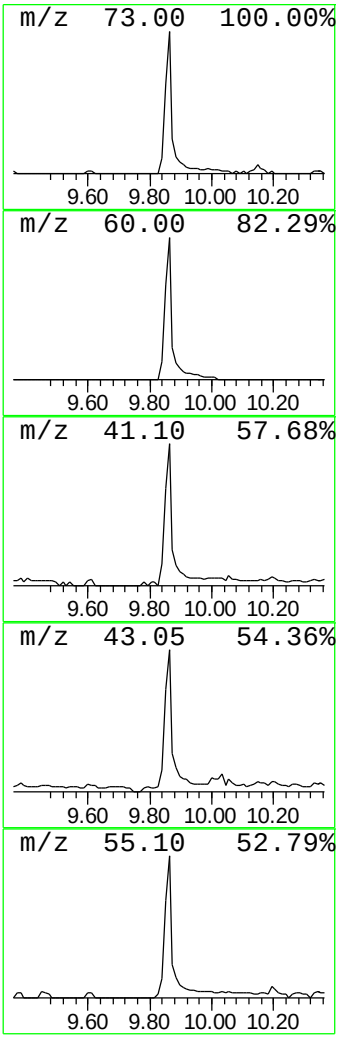
****

Peak Number 8 Dodecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	10.67 ng	244744	Acenaphthene-d10	9.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	91
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	Octanoic acid	144	C8H16O2	000124-07-2	43
4	Nonanoic acid	158	C9H18O2	000112-05-0	43
5	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	10





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Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

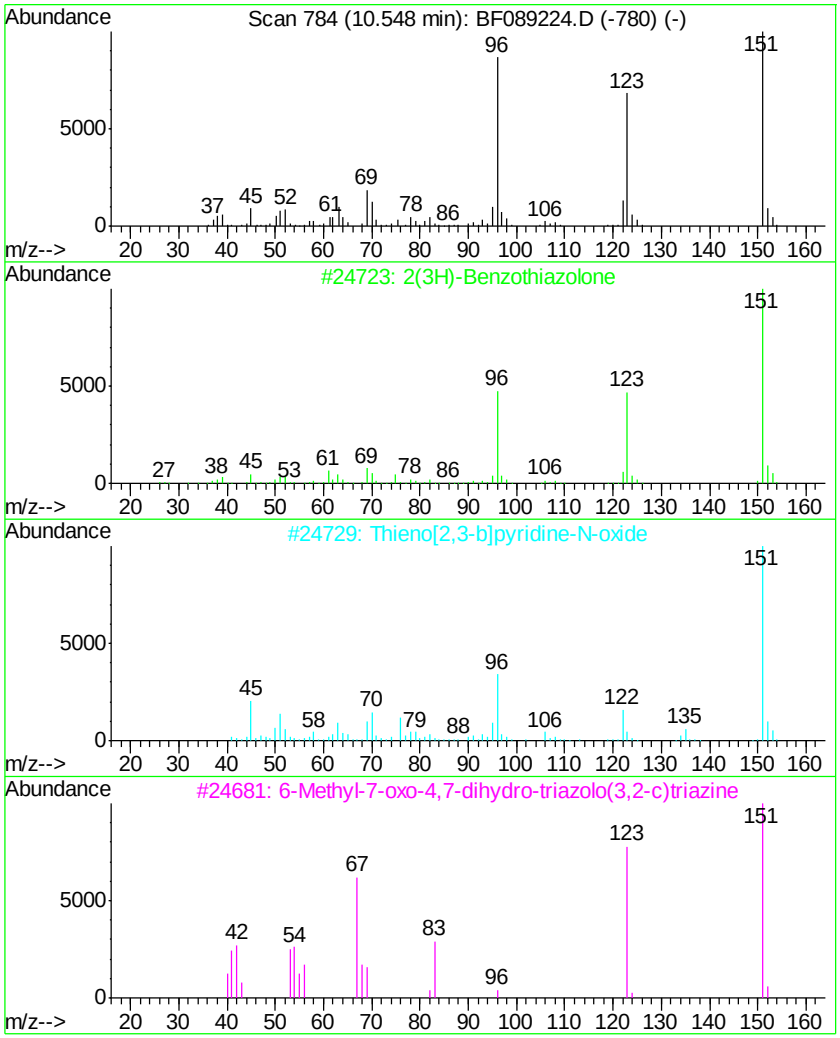
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

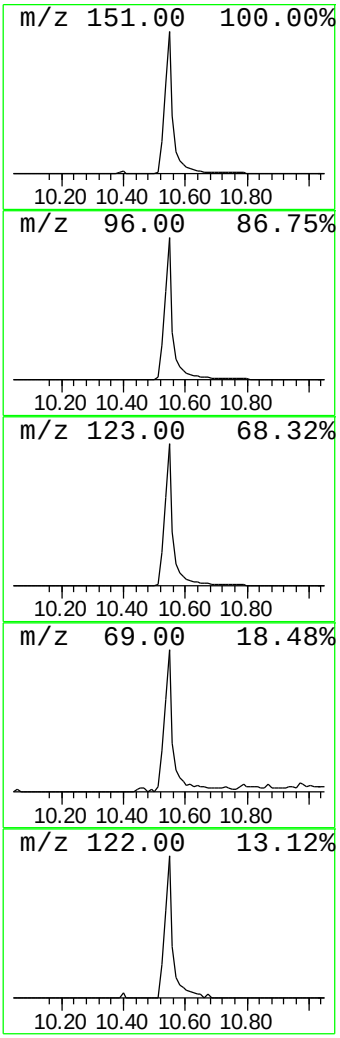
****

Peak Number 9 2(3H)-Benzothiazolone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	30.74 ng	713579	Phenanthrene-d10	11.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	95
2	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	43
3	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	43
4	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	38
5	5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	30





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Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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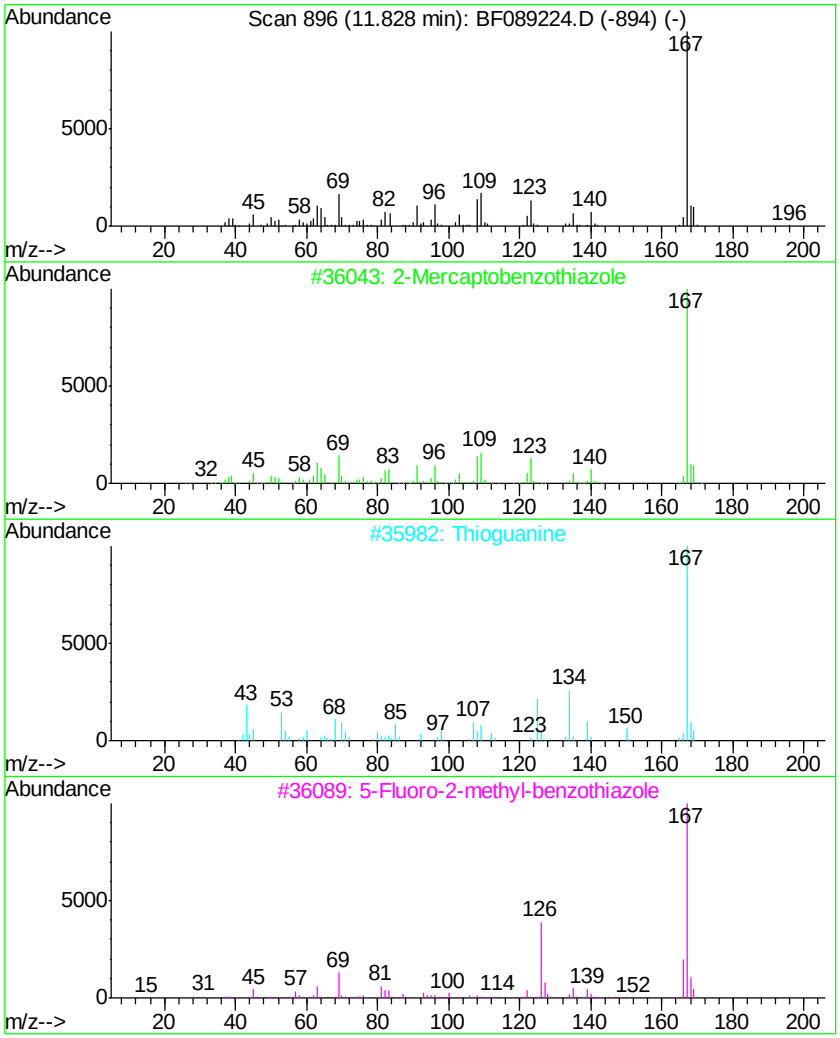
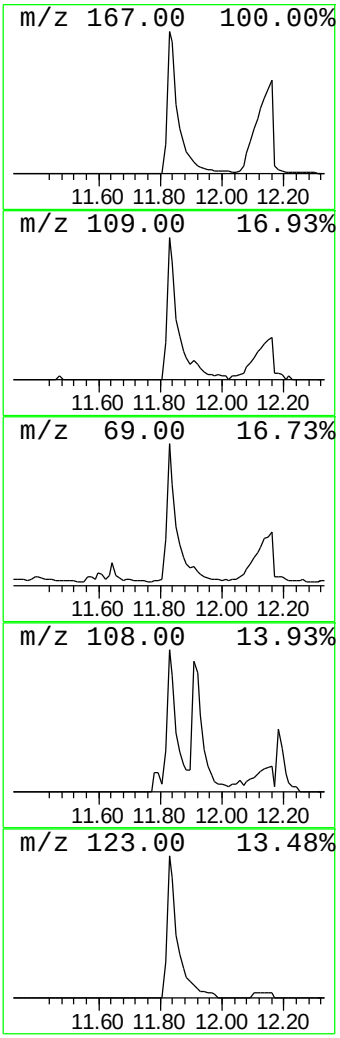
Peak Number 10 2-Mercaptobenzothiazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	26.75 ng	620972	Phenanthrene-d10	11.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	97
2	Thioguanine	167	C5H5N5S	000154-42-7	53
3	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	50
4	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	47
5	3-Methoxythiobenzamide	167	C8H9NOS	064559-06-4	45





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Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

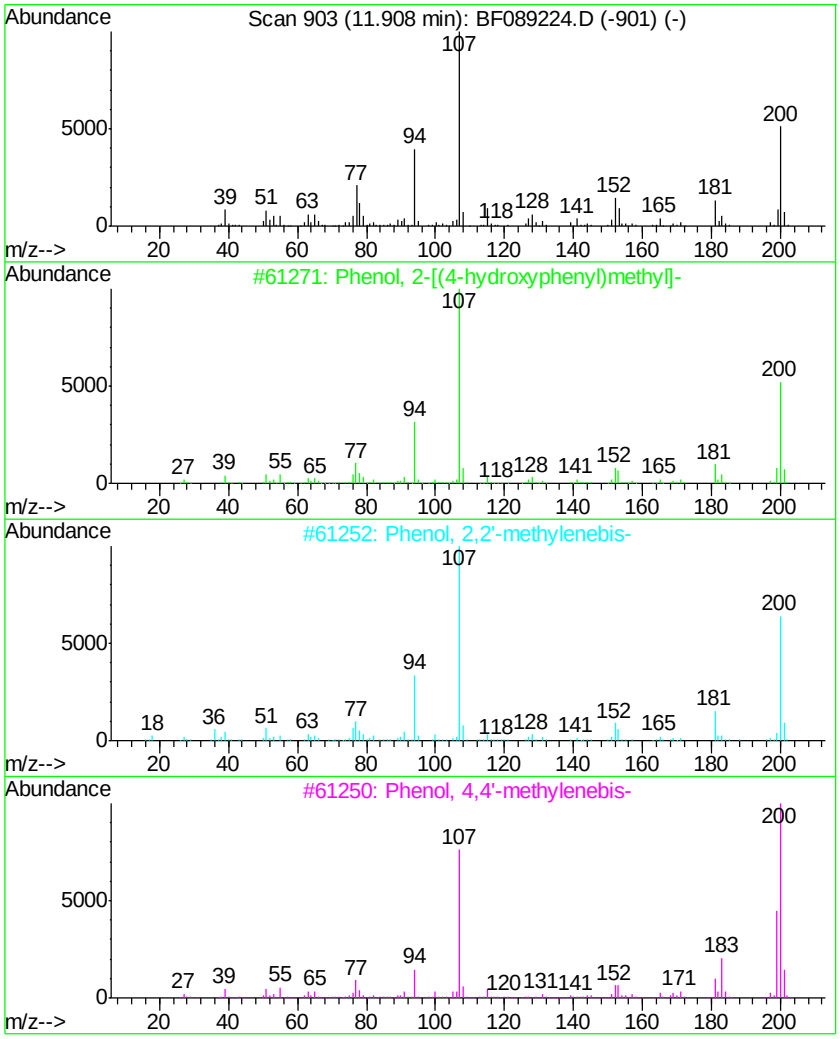
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

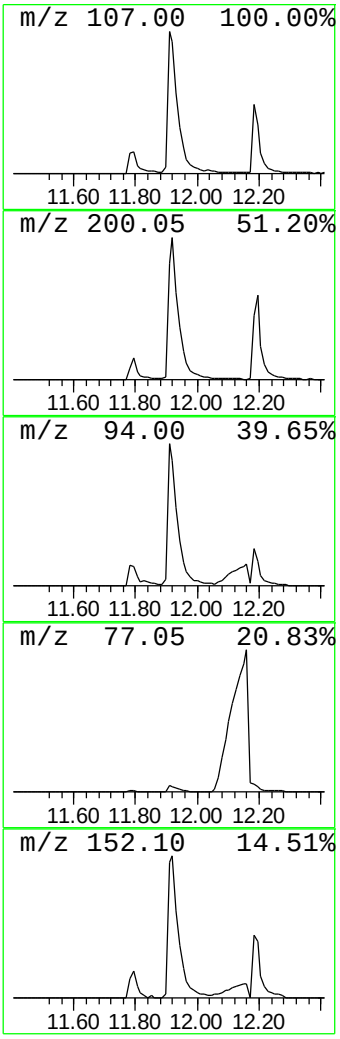
****

Peak Number 11 Phenol, 2-[(4-hydroxyphenyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	55.38 ng	1285520	Phenanthrene-d10	11.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	97
2	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	94
3	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	68
4	Ethyl 2-hydroxybenzyl sulfone	200	C9H12O3S	053380-27-1	49
5	4-(2-Methoxyethyl)phenol	152	C9H12O2	056718-71-9	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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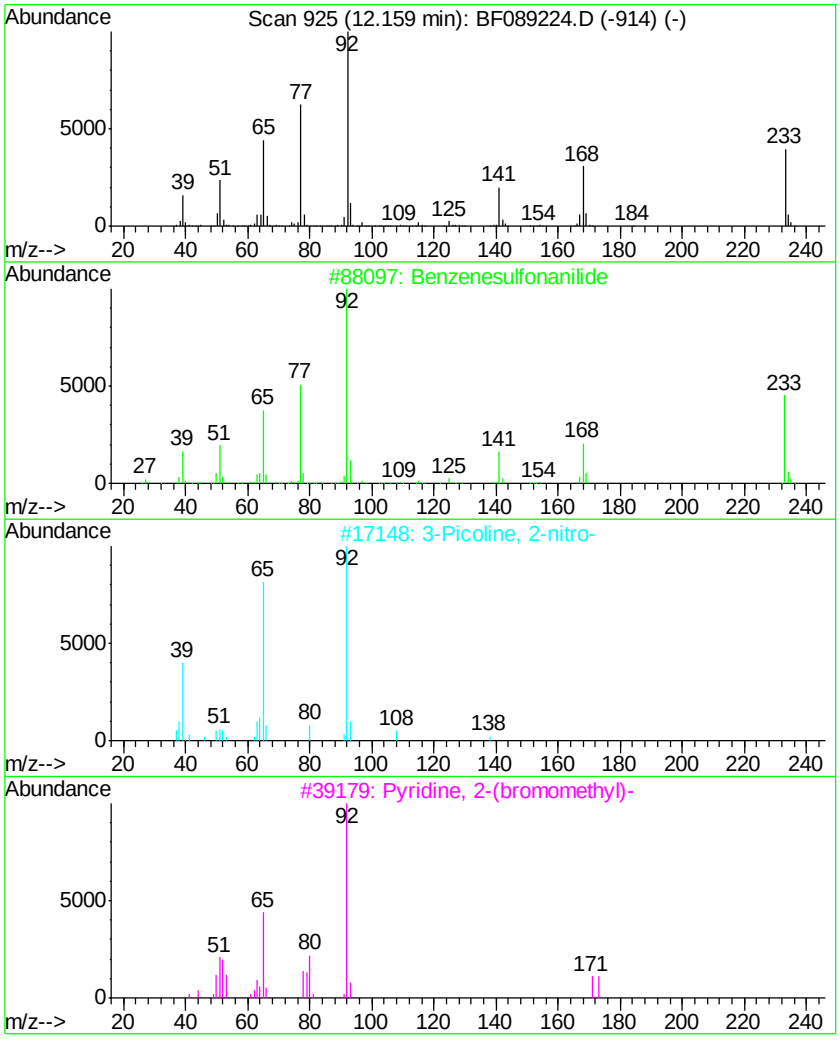
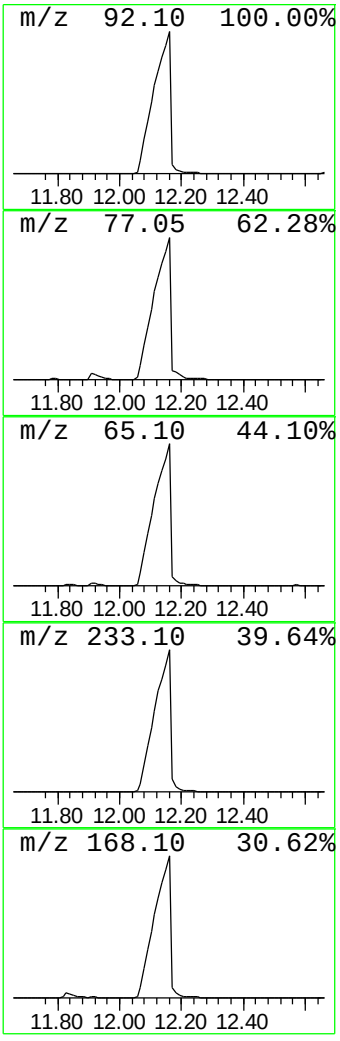
****

Peak Number 12 Benzenesulfonanilide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	548.05 ng	12722900	Phenanthrene-d10	11.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonanilide	233	C12H11NO2S	001678-25-7	98
2	3-Picoline, 2-nitro-	138	C6H6N2O2	018368-73-5	47
3	Pyridine, 2-(bromomethyl)-	171	C6H6BrN	055401-97-3	40
4	Methanesulfanilide	171	C7H9NO2S	001197-22-4	32
5	N-(4-Bromophenylsulfonyl)-1H-aze...	311	C12H10BrNO2S	020646-55-3	28





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Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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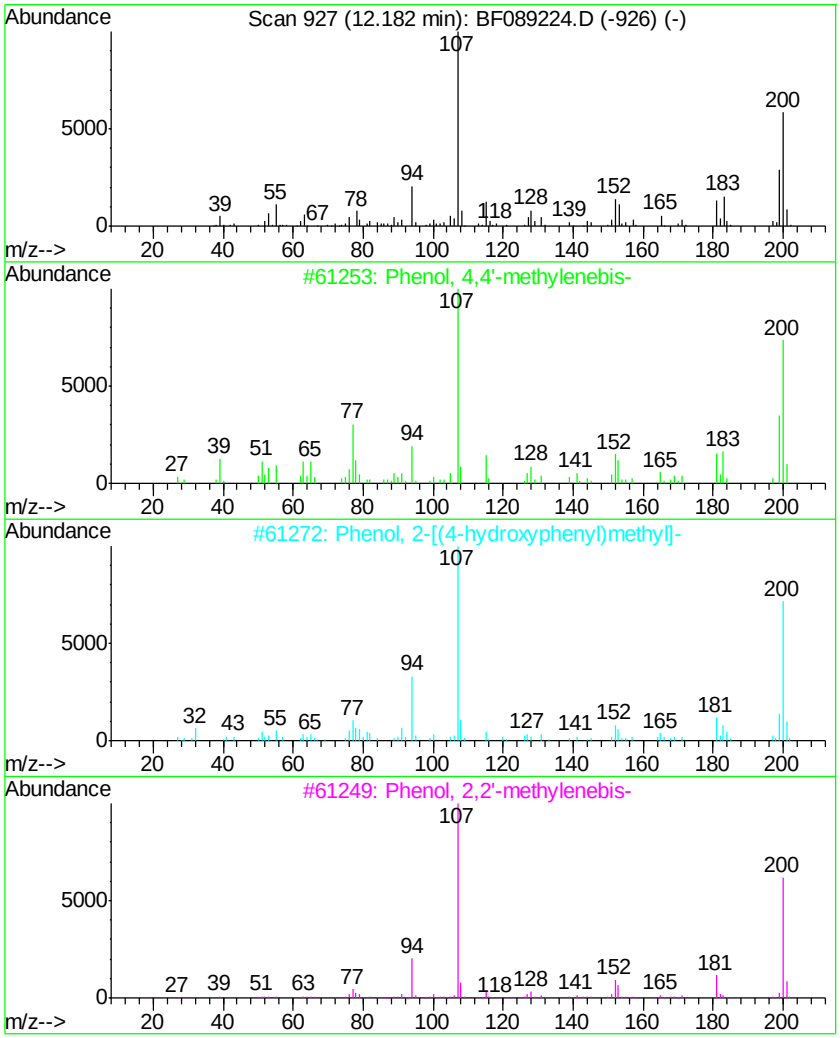
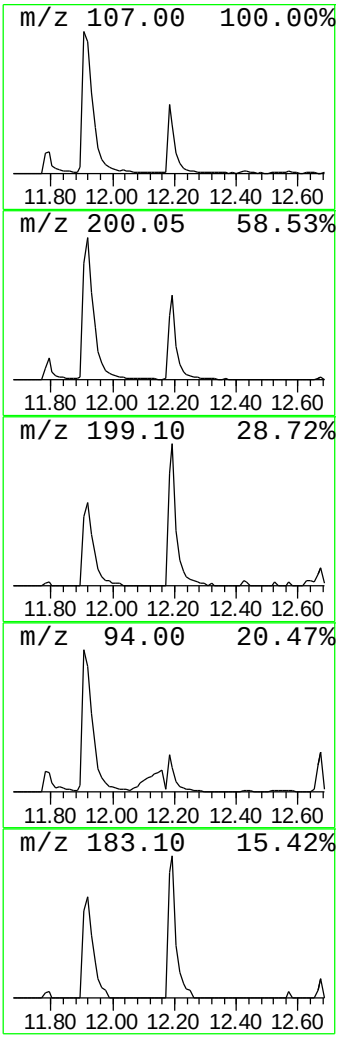
Peak Number 13 Phenol, 4,4'-methylenebis- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.18	30.98 ng	719112	Phenanthrene-d10	11.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	98
2	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	91
3	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	87
4	1,3-Benzenediol, 4-(phenylmethyl)-	200	C13H12O2	002284-30-2	46
5	Phosphine, methyldiphenyl-	200	C13H13P	001486-28-8	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

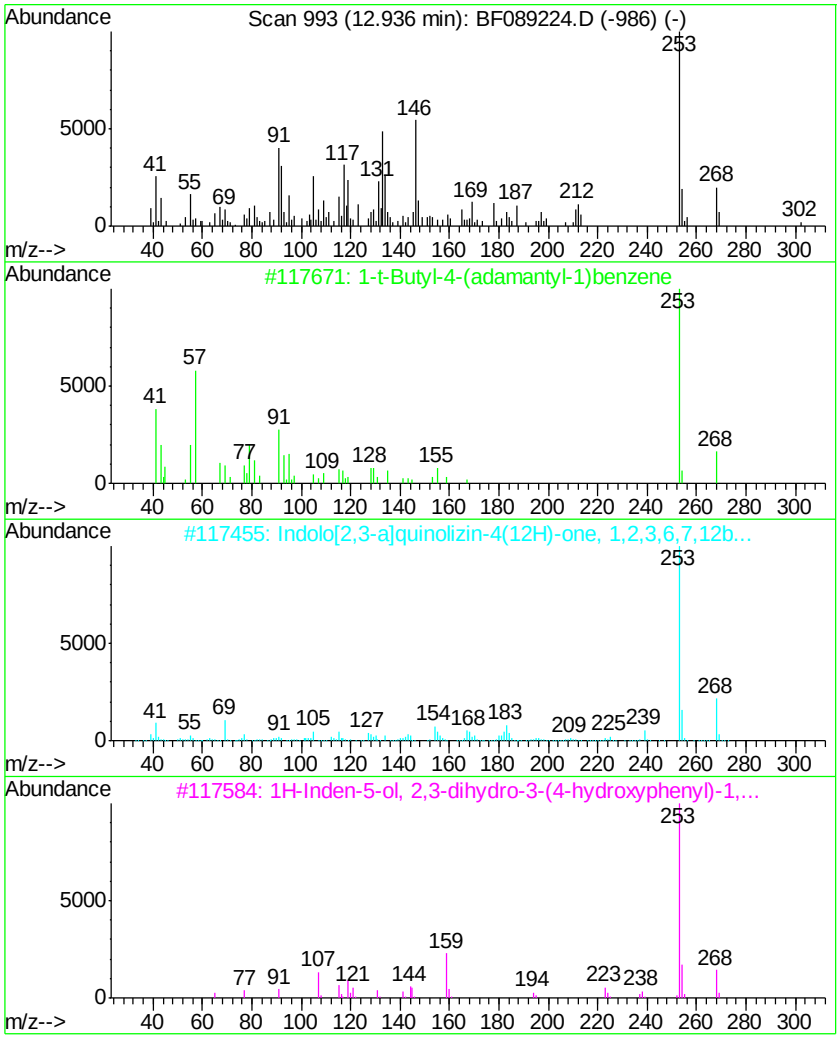
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

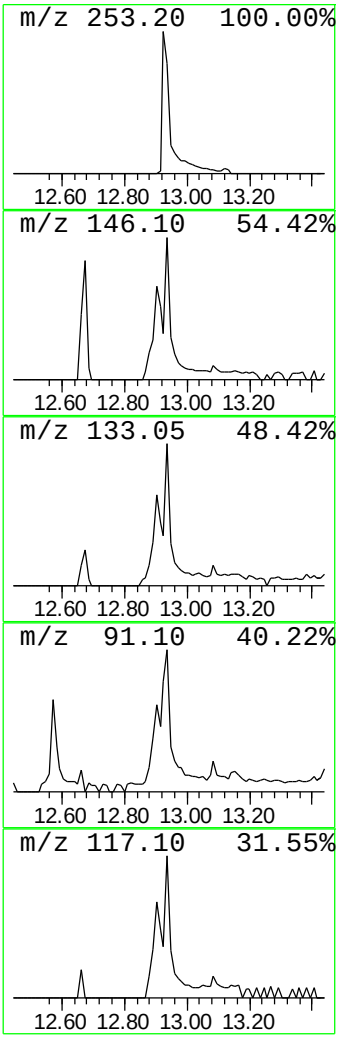
****

Peak Number 14 unknown12.94 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	21.86 ng	406887	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-t-Butyl-4-(adamantyl-1)benzene	268	C20H28	059974-45-7	38
2	Indolo[2,3-a]quinolizin-4(12H)-o...	268	C17H20N2O	020156-09-6	38
3	1H-Inden-5-ol, 2,3-dihydro-3-(4-...	268	C18H20O2	010527-11-4	38
4	9,10-Anthracenedione, 1,8-dimeth...	268	C16H12O4	006407-55-2	27
5	Phenol, 4-methyl-2--(4-isopropyl...	253	C17H19NO	315671-87-5	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089224.D
Acq On : 23 Jul 2016 8:23
Operator : UM/SJ
Sample : H4121-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-TEMP-MW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
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
unknown6.34	6.34	92.0	ng	1202670	1	6.58	261574	20.0
1-Hexanol, 2-ethyl-	6.66	60.4	ng	790054	1	6.58	261574	20.0
Hexanoic acid, 2-...	7.35	18.3	ng	392236	2	7.86	428065	20.0
Ethanol, 2-(2-but...	7.79	6.0	ng	128911	2	7.86	428065	20.0
Benzothiazole	8.15	53.6	ng	1147110	2	7.86	428065	20.0
Dodecanoic acid	9.86	10.7	ng	244744	3	9.61	458822	20.0
2(3H)-Benzothiazo...	10.55	30.7	ng	713579	4	11.08	464295	20.0
2-Mercaptobenzoth...	11.83	26.8	ng	620972	4	11.08	464295	20.0
Phenol, 2-[(4-hyd...	11.91	55.4	ng	1285520	4	11.08	464295	20.0
Benzenesulfonanilide	12.16	548.0	ng	12722900	4	11.08	464295	20.0
Phenol, 4,4'-meth...	12.18	31.0	ng	719112	4	11.08	464295	20.0
unknown12.94	12.94	21.9	ng	406887	5	13.70	372201	20.0