LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

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-BF112316.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	1.767	5	7	17	rVB	567946	1139711	11.19%	1.540%
2	1.904	17	19	67	rVB	4345654	10186071	100.00%	13.763%
3	5.059	292	295	297	rBV	565444	699235	6.86%	0.945%
4	5.470	328	331	333	rBV	2829817	2597190	25.50%	3.509%
5	5.733	351	354	357	rBV	414379	371863	3.65%	0.502%
6	6.316	403	405	407	rVB	116476	103086	1.01%	0.139%
7	6.487	418	420	423	rVB	1367077	1553542	15.25%	2.099%
8	6.636	430	433	436	rBV	3627183	4450699	43.69%	6.014%
9	6.876	451	454	456	rBV	1479642	1269779	12.47%	1.716%
10	6.945	457	460	463	rBV	5469306	8421513	82.68%	11.379%
11	7.036	465	468	470	rVB	4584690	4516848	44.34%	6.103%
12	7.436	500	503	505	rBV	3275910	3417824	33.55%	4.618%
13	7.539	508	512	514	rBV	198553	325934	3.20%	0.440%
14	8.156	564	566	569	rBV	1540666	1600414	15.71%	2.162%
15	8.430	588	590	593	rVB	259330	243135	2.39%	0.329%
16	8.796	618	622	624	rBV	1601926	1985239	19.49%	2.682%
17	8.922	630	633	635	rBV	214777	299211	2.94%	0.404%
18	9.242	658	661	663	rBV	6489050	6587650	64.67%	8.901%
19	9.916	717	720	722	rVB	2119936	1971191	19.35%	2.663%
20	10.545	772	775	777	rBV	223216	189301	1.86%	0.256%
21	10.705	785	789	791	rBV	3903623	4592669	45.09%	6.205%
22	11.402	847	850	852	rVB	1485383	1959093	19.23%	2.647%
23	11.928	894	896	898	rBV	134701	159374	1.56%	0.215%
24	11.962	898	899	902	rVB	427260	472817	4.64%	0.639%
25	12.099	908	911	917	rBV	139675	253356	2.49%	0.342%
26	12.374	932	935	937	rBV	101065	148895	1.46%	0.201%
27	12.591	950	954	957	rBV	2204952	3899042	38.28%	5.268%
28	12.728	964	966	969	rBV	177471	280209	2.75%	0.379%
29	12.991	986	989	991	rBV	6605724	6724715	66.02%	9.086%
30	14.031	1077	1080	1082	rBV	2085384	1950092	19.14%	2.635%
31	15.471	1202	1206	1209	rBV	1107263	1503890	14.76%	2.032%
32	16.191	1262	1269	1277	rBV3	25897	137216	1.35%	0.185%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

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-BF112316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

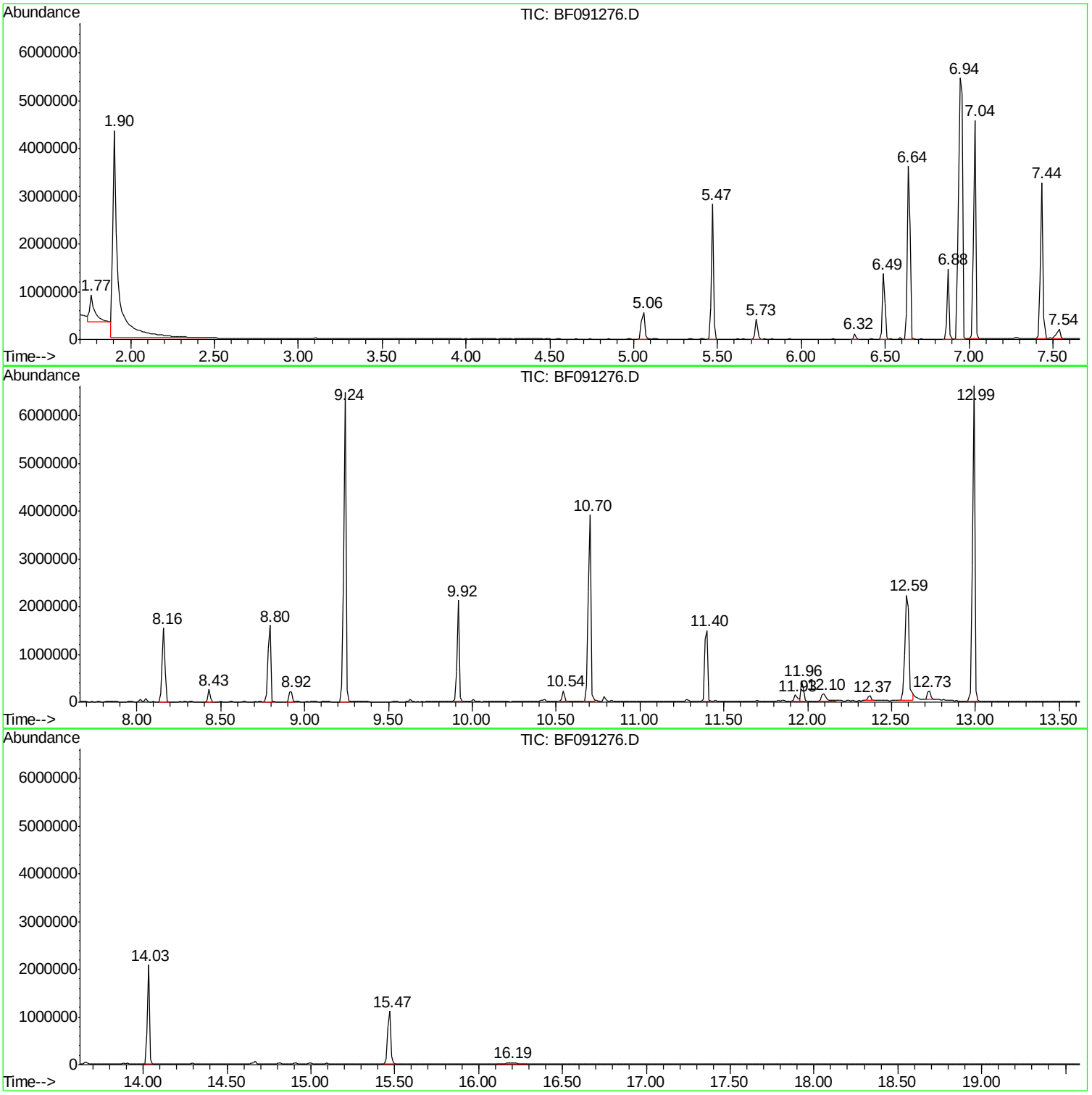
Sum of corrected areas: 74010804

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.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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Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

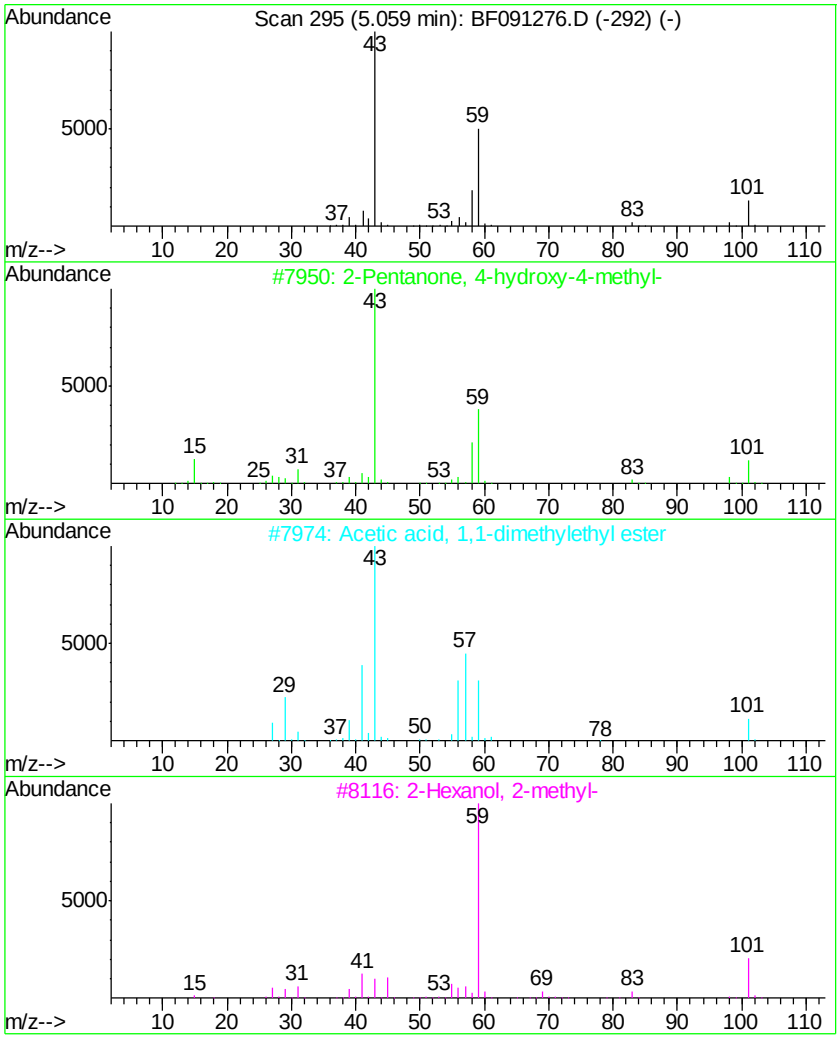
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

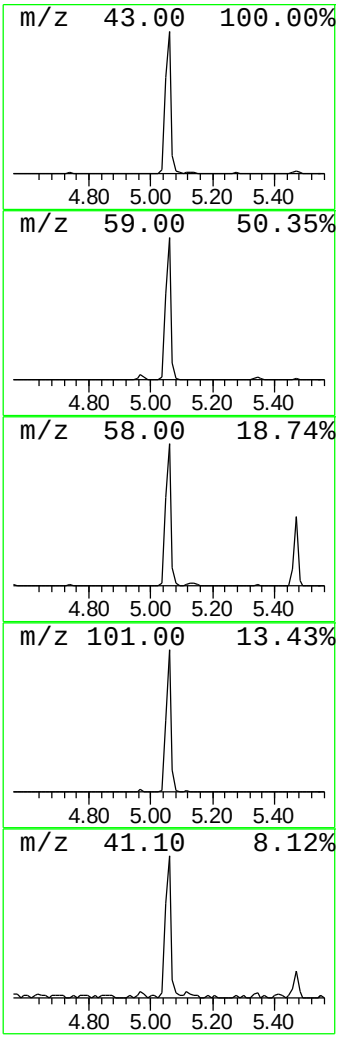
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	11.01 ng	699235	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

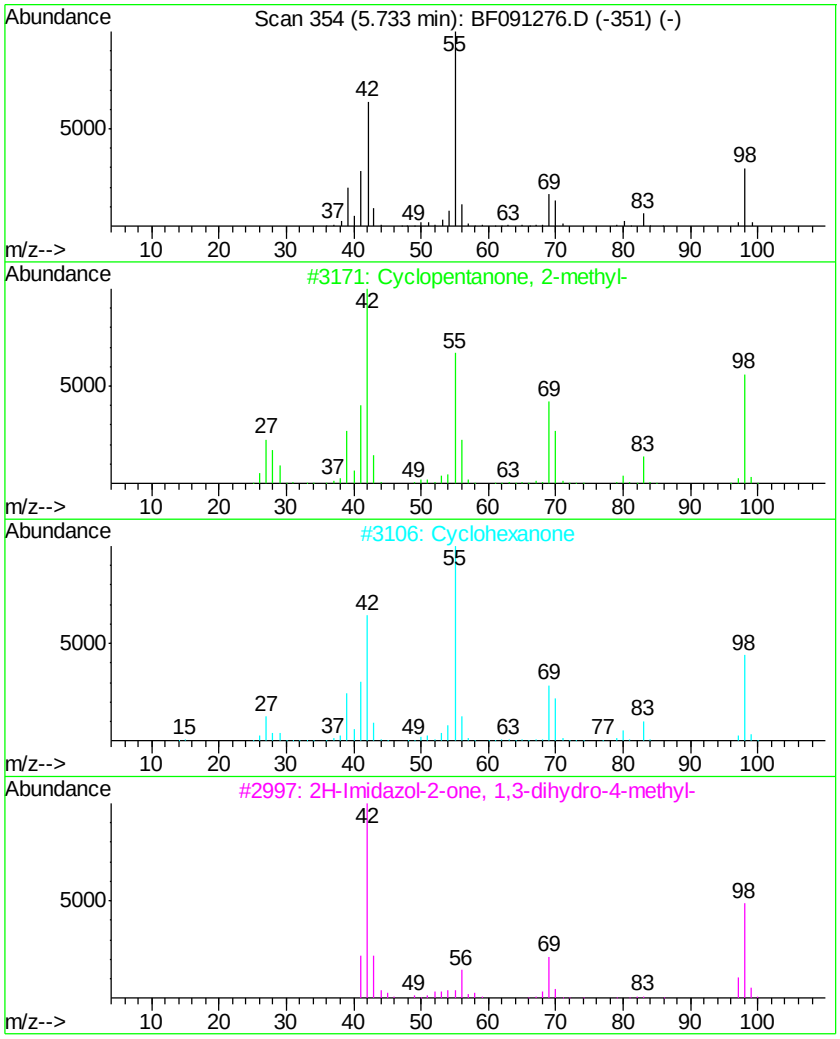
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

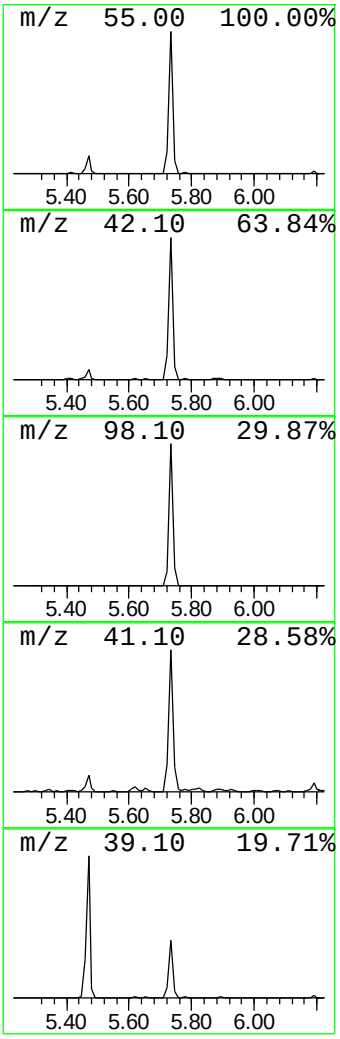
****

Peak Number 4 Cyclopentanone, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	5.86 ng	371863	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	80
2	Cyclohexanone	98	C6H10O	000108-94-1	70
3	2H-Imidazol-2-one, 1,3-dihydro-4...	98	C4H6N2O	001192-34-3	36
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	35
5	2(5H)-Furanone, 5-methyl-	98	C5H6O2	000591-11-7	32





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.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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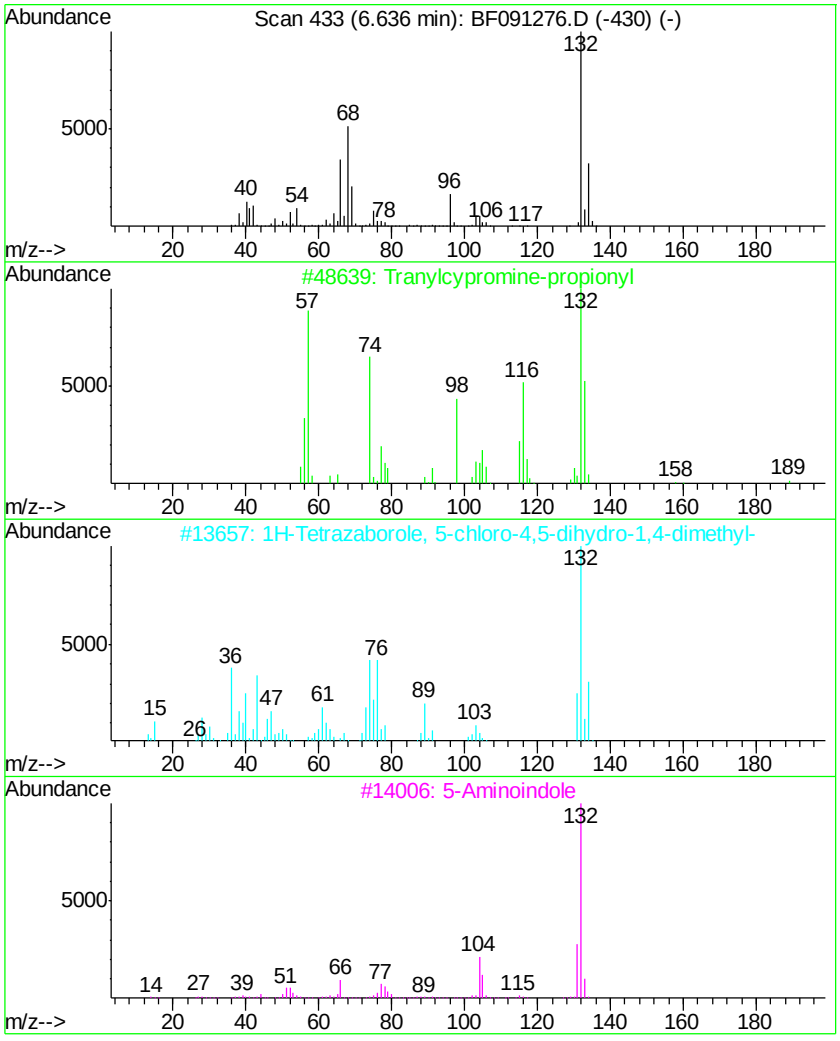
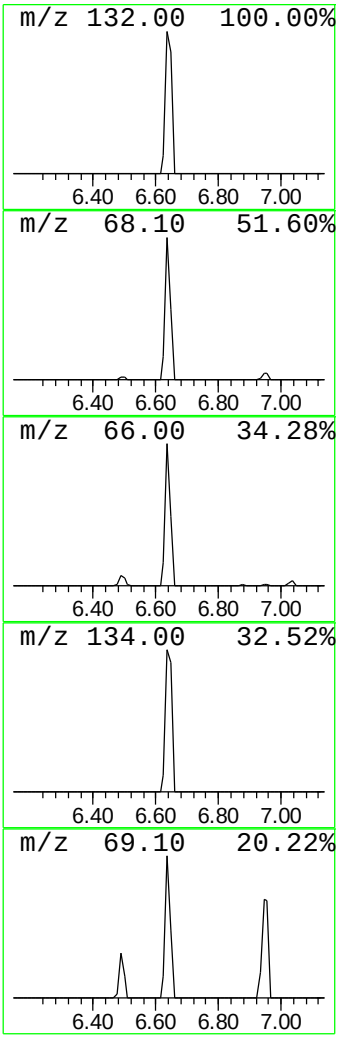
Peak Number 5 unknown6.64 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	70.10 ng	4450700	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
2	1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
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\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

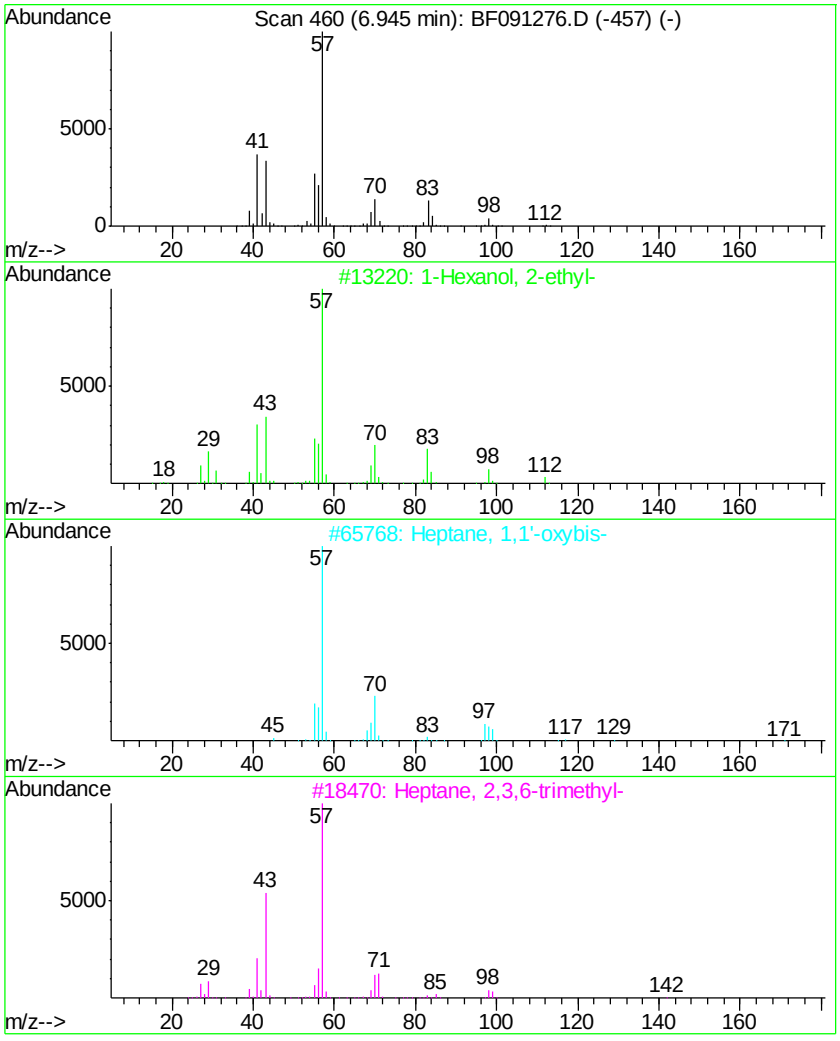
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

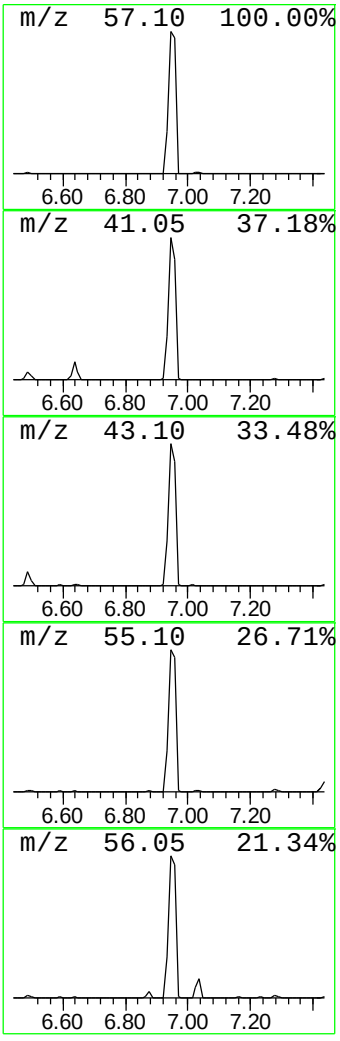
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	132.65 ng	8421510	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3	Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
4	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

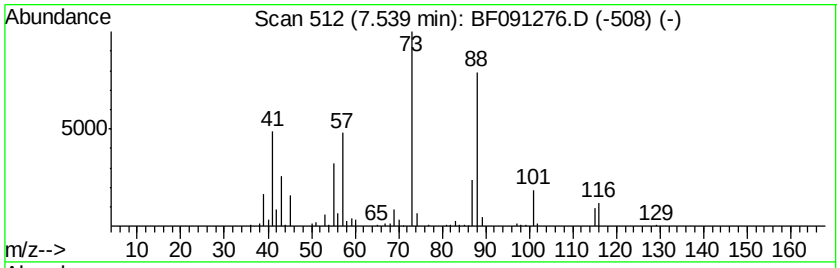
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

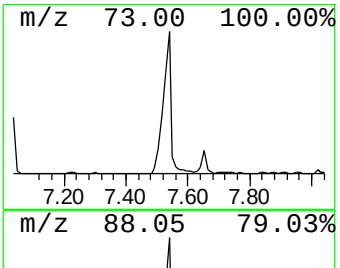
****

Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	4.07 ng	325934	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	50
4	1,4-Dioxane	88	C4H8O2	000123-91-1	47
5	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42





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Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

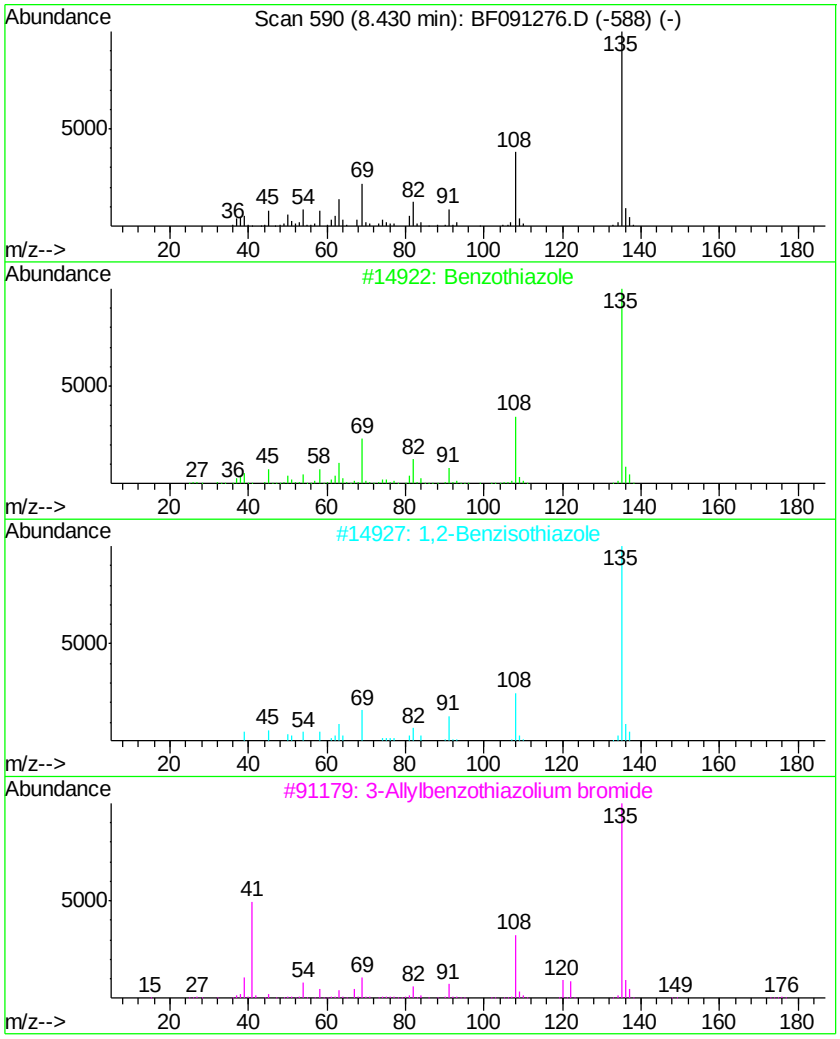
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

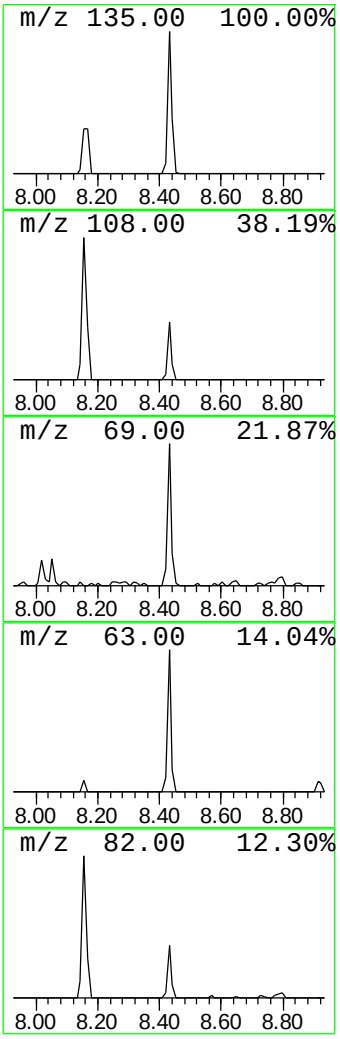
****

Peak Number 9 Benzothiazole Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.43	3.04 ng	243135	Naphthalene-d8	8.16

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	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	78
4	Adenine	135	C5H5N5	000073-24-5	64
5	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

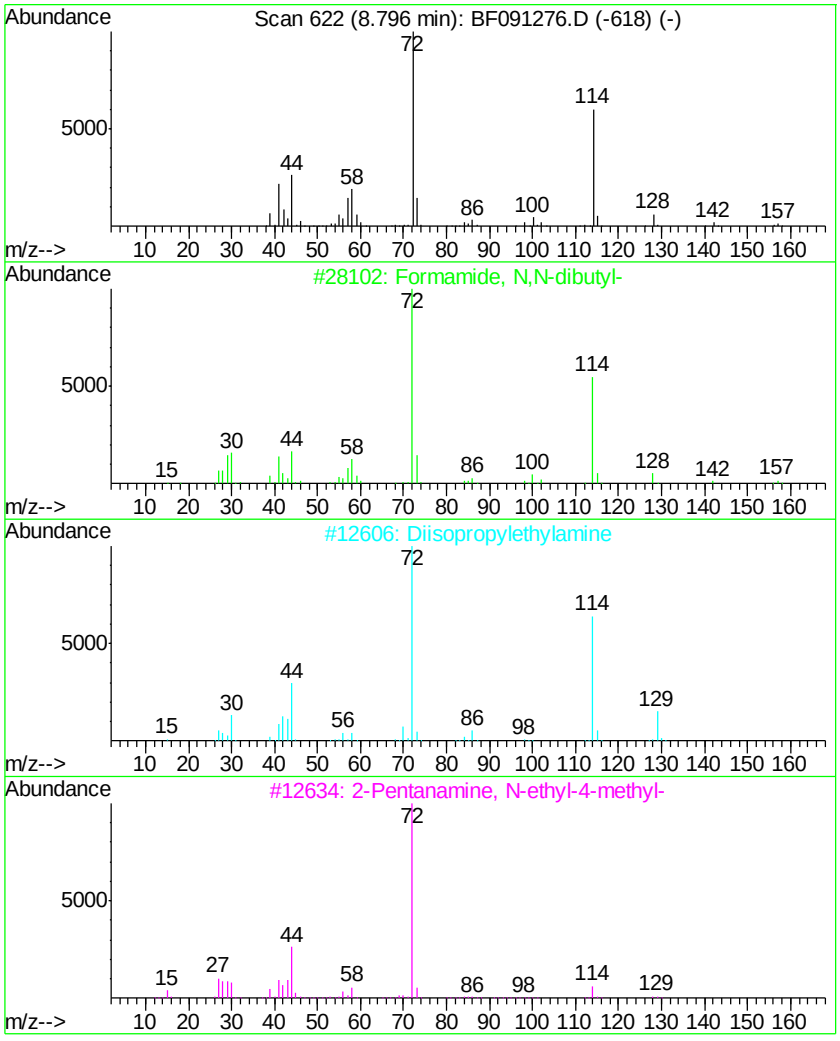
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

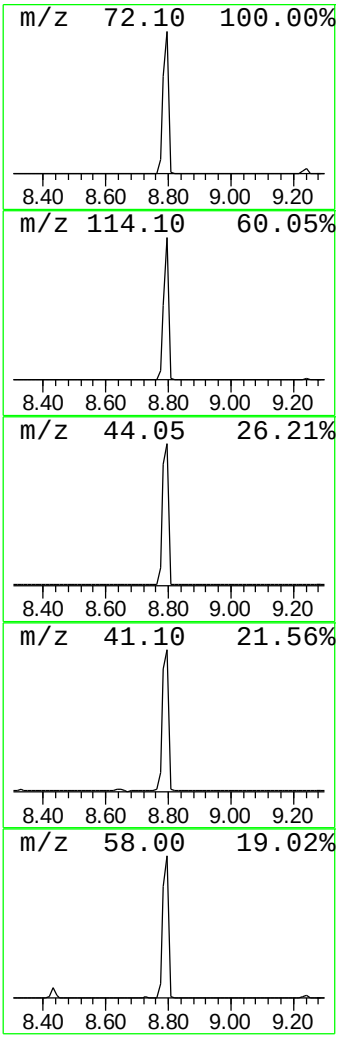
****

Peak Number 10 Formamide, N,N-dibutyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	24.81 ng	1985240	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formamide, N,N-dibutyl-	157	C9H19NO	000761-65-9	90
2	Diisopropylethylamine	129	C8H19N	007087-68-5	50
3	2-Pentanamine, N-ethyl-4-methyl-	129	C8H19N	042966-64-3	47
4	Dimethyl(2-octyl)amine	157	C10H23N	007378-97-4	43
5	1-Butanamine, N-(1-methylethyl)-	115	C7H17N	039099-23-5	40





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Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

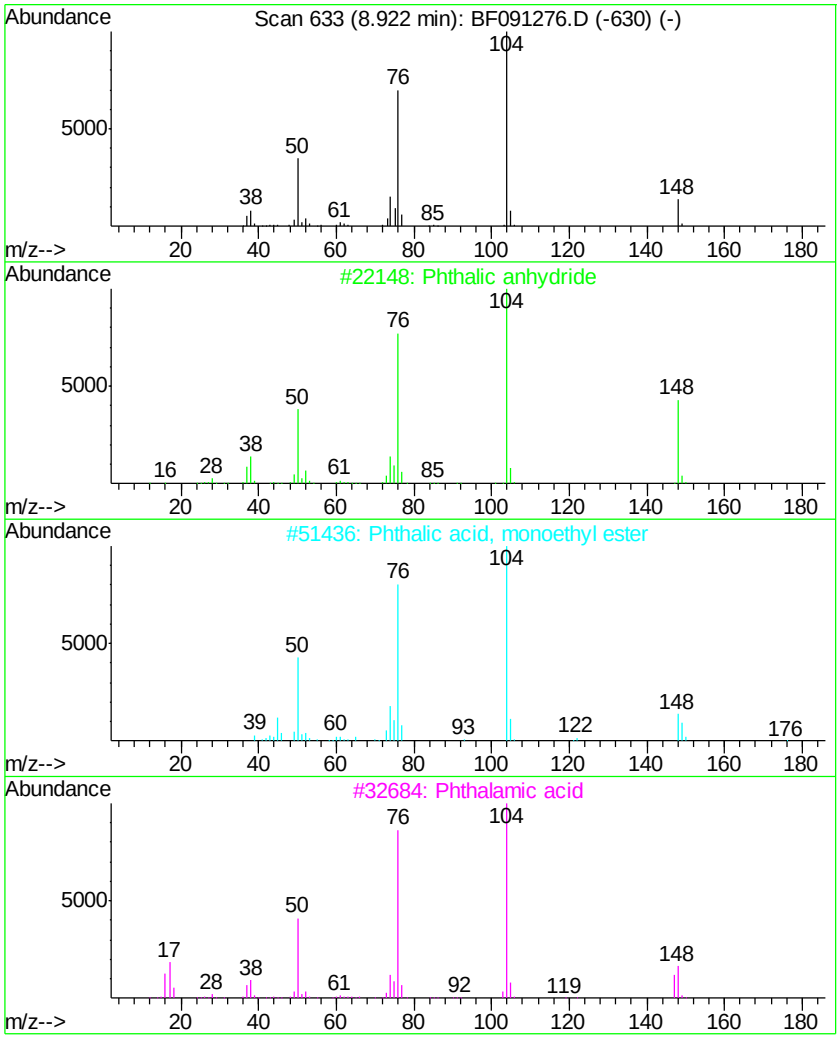
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

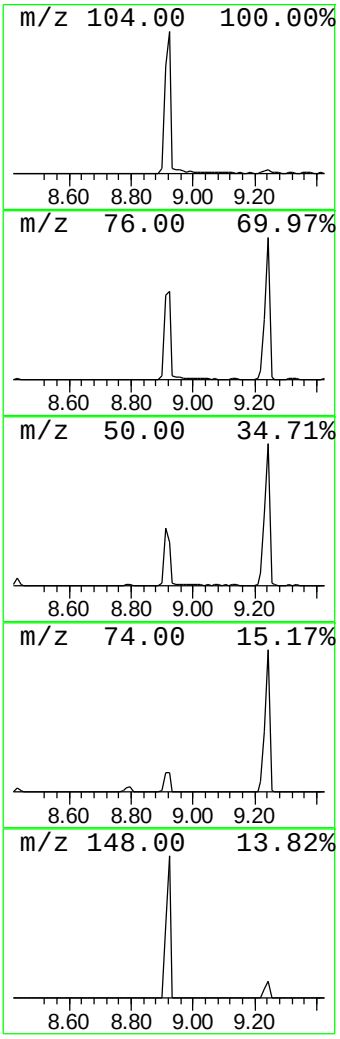
****

Peak Number 11 Phthalic anhydride Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.92	3.74 ng	299211	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	95
2	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	90
3	Phthalamic acid	165	C8H7NO3	000088-97-1	83
4	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83
5	N-[2-Acetamidoethylthio]phthalimide	264	C12H12N2O3S	025158-14-9	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

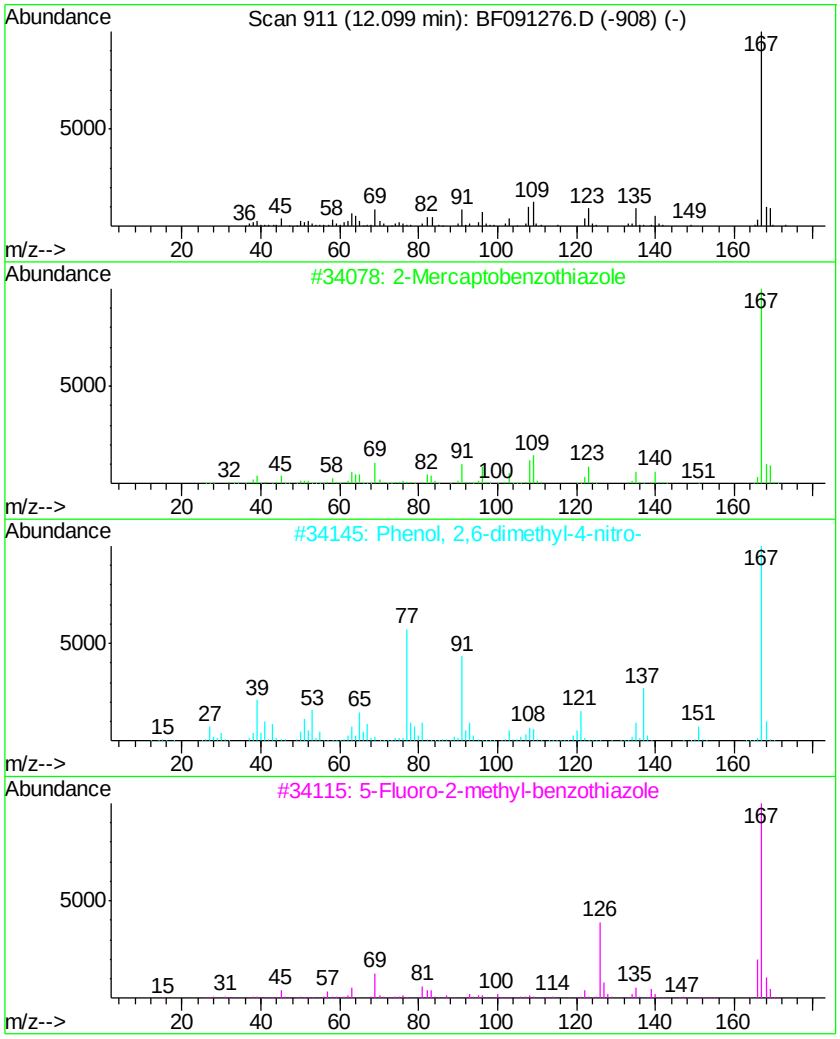
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

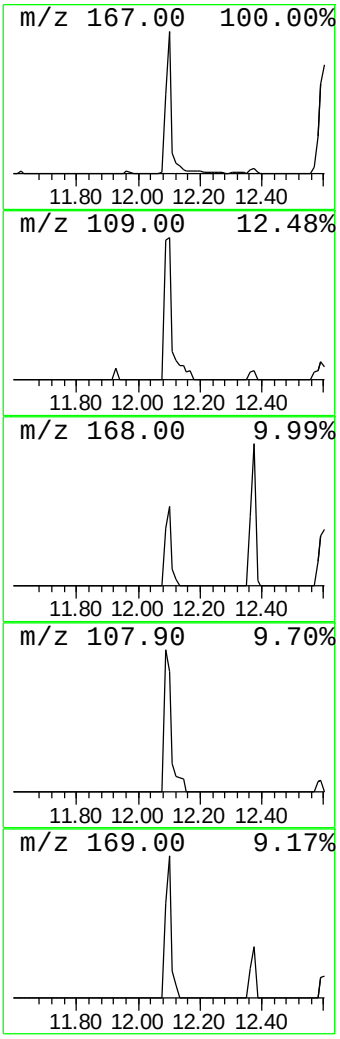
****

Peak Number 12 2-Mercaptobenzothiazole Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.10	2.59 ng	253356	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
2	Phenol, 2,6-dimethyl-4-nitro-	167	C8H9NO3	002423-71-4	59
3	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	50
4	3-Methoxythiobenzamide	167	C8H9NOS	064559-06-4	45
5	Thioguanine	167	C5H5N5S	000154-42-7	42





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Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

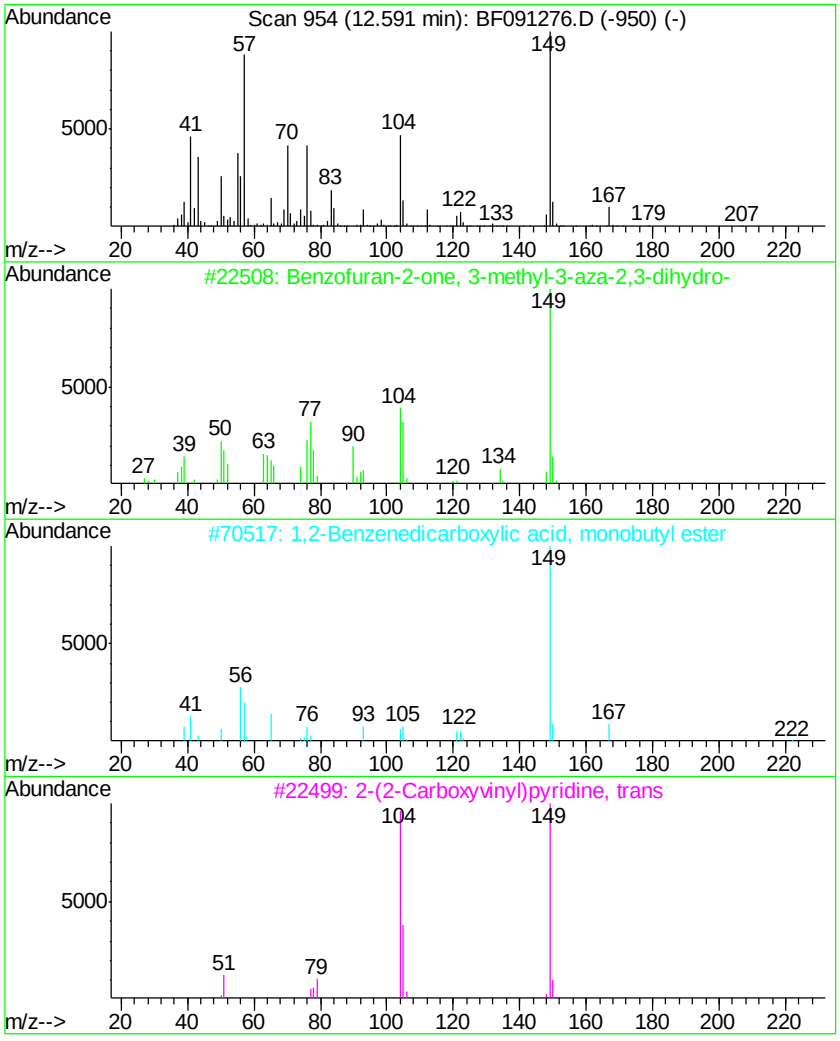
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

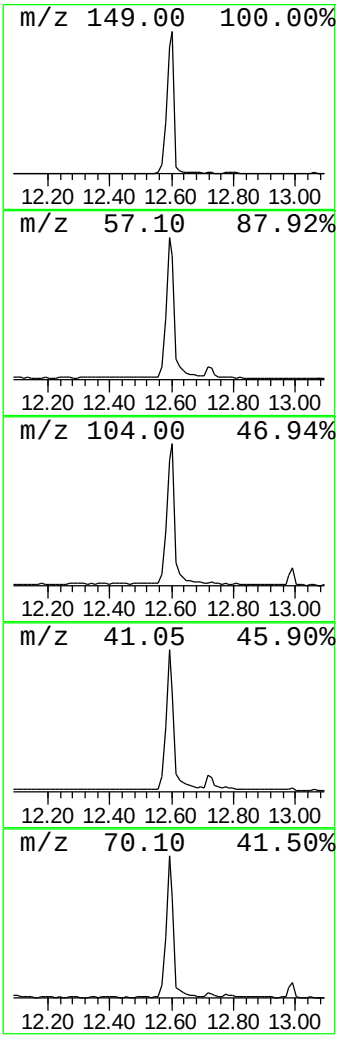
****

Peak Number 13 unknown12.59 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	39.80 ng	3899040	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran-2-one, 3-methyl-3-aza...	149	C8H7NO2	1000289-12-2	43
2	1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	38
3	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	25
4	Phthalic acid, 2-hexyl ester	250	C14H18O4	079107-80-5	25
5	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	16





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

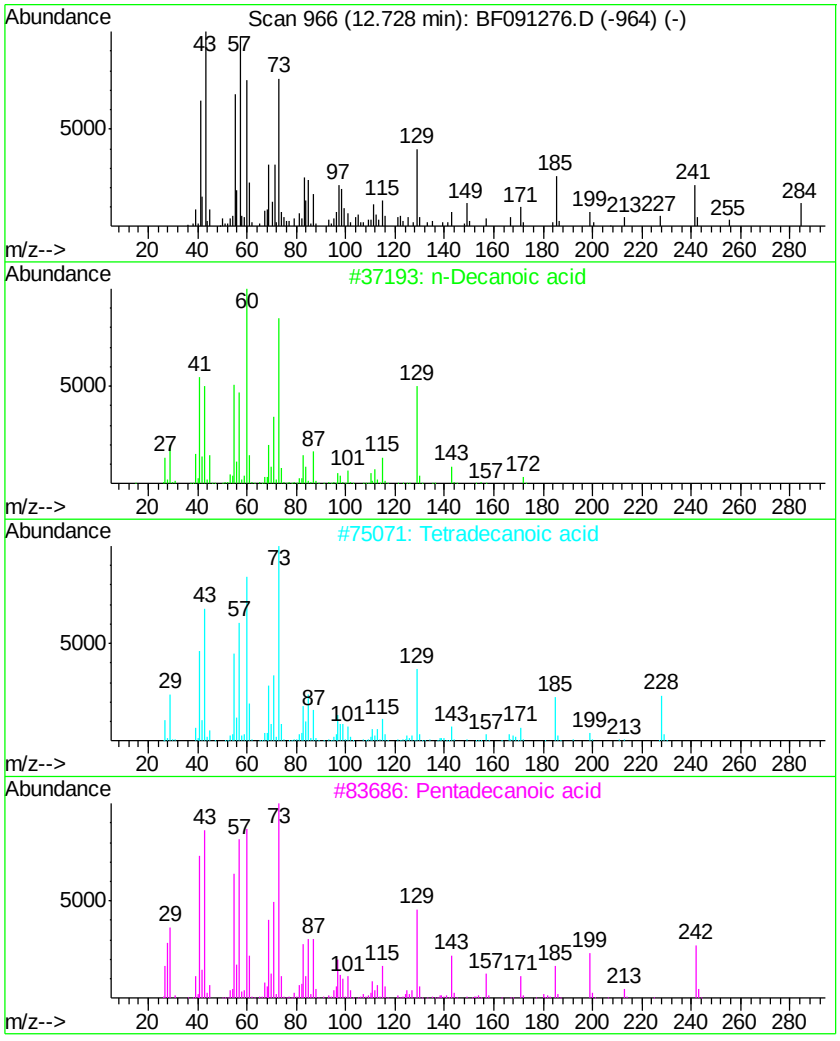
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

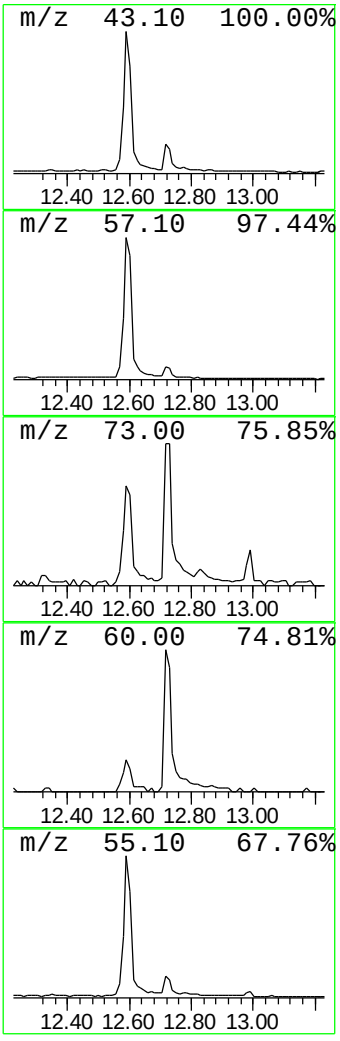
****

Peak Number 14 n-Decanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.87 ng	280209	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	87
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Undecanoic acid	186	C11H22O2	000112-37-8	49
5	Tridecanoic acid	214	C13H26O2	000638-53-9	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112316\
Data File : BF091276.D
Acq On : 23 Nov 2016 15:23
Operator : UM/SJ
Sample : H5747-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DW-BSB-11222016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112316.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-Pentanone, 4-hy...	5.06	11.0	ng	699235	1	6.88	1269780	20.0
Cyclopentanone, 2...	5.73	5.9	ng	371863	1	6.88	1269780	20.0
unknown6.64	6.64	70.1	ng	4450700	1	6.88	1269780	20.0
1-Hexanol, 2-ethyl-	6.94	132.7	ng	8421510	1	6.88	1269780	20.0
Hexanoic acid, 2-...	7.54	4.1	ng	325934	2	8.16	1600410	20.0
Benzothiazole	8.43	3.0	ng	243135	2	8.16	1600410	20.0
Formamide, N,N-di...	8.80	24.8	ng	1985240	2	8.16	1600410	20.0
Phthalic anhydride	8.92	3.7	ng	299211	2	8.16	1600410	20.0
2-Mercaptobenzoth...	12.10	2.6	ng	253356	4	11.40	1959090	20.0
unknown12.59	12.59	39.8	ng	3899040	4	11.40	1959090	20.0
n-Decanoic acid	12.73	2.9	ng	280209	5	14.03	1950090	20.0