LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075594.D
Acq On : 16 Nov 2014 22:05
Operator : TP / JJ
Sample : F4742-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DCW-WW-021-111214

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-BF111214.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	1.361	22	24	26	rBV	716112	972706	3.90%	1.832%
2	1.773	56	60	64	rVB	190569	298246	1.20%	0.562%
3	1.967	73	77	101	rVB2	796293	1586623	6.36%	2.989%
4	6.184	442	446	448	rBV	3458051	4677767	18.76%	8.812%
5	7.270	538	541	543	rVB	504335	620619	2.49%	1.169%
6	7.693	571	578	580	rBV	9453671	24938989	100.00%	46.981%
7	7.739	580	582	584	rVV	562863	725838	2.91%	1.367%
8	8.242	624	626	629	rVB	497377	562674	2.26%	1.060%
9	8.447	634	644	647	rBV	378736	1235890	4.96%	2.328%
10	9.133	702	704	706	rVB	318970	271098	1.09%	0.511%
11	9.476	732	734	737	rBV	586044	672742	2.70%	1.267%
12	10.482	819	822	824	rBV	1358631	1428731	5.73%	2.691%
13	11.316	892	895	897	rBV	397835	393465	1.58%	0.741%
14	12.299	978	981	986	rVB2	882332	1262029	5.06%	2.377%
15	12.448	990	994	997	rBV	519150	775879	3.11%	1.462%
16	13.168	1054	1057	1059	rVB	346935	386131	1.55%	0.727%
17	13.397	1071	1077	1080	rBV	4023093	9440431	37.85%	17.784%
18	13.454	1080	1082	1098	rVB	282179	542097	2.17%	1.021%
19	14.071	1134	1136	1139	rBV	250675	372388	1.49%	0.702%
20	15.157	1228	1231	1234	rBV	1148192	1206393	4.84%	2.273%
21	16.460	1342	1345	1351	rVB	363260	387102	1.55%	0.729%
22	18.231	1497	1500	1503	rBV	222139	325332	1.30%	0.613%

Sum of corrected areas: 53083170

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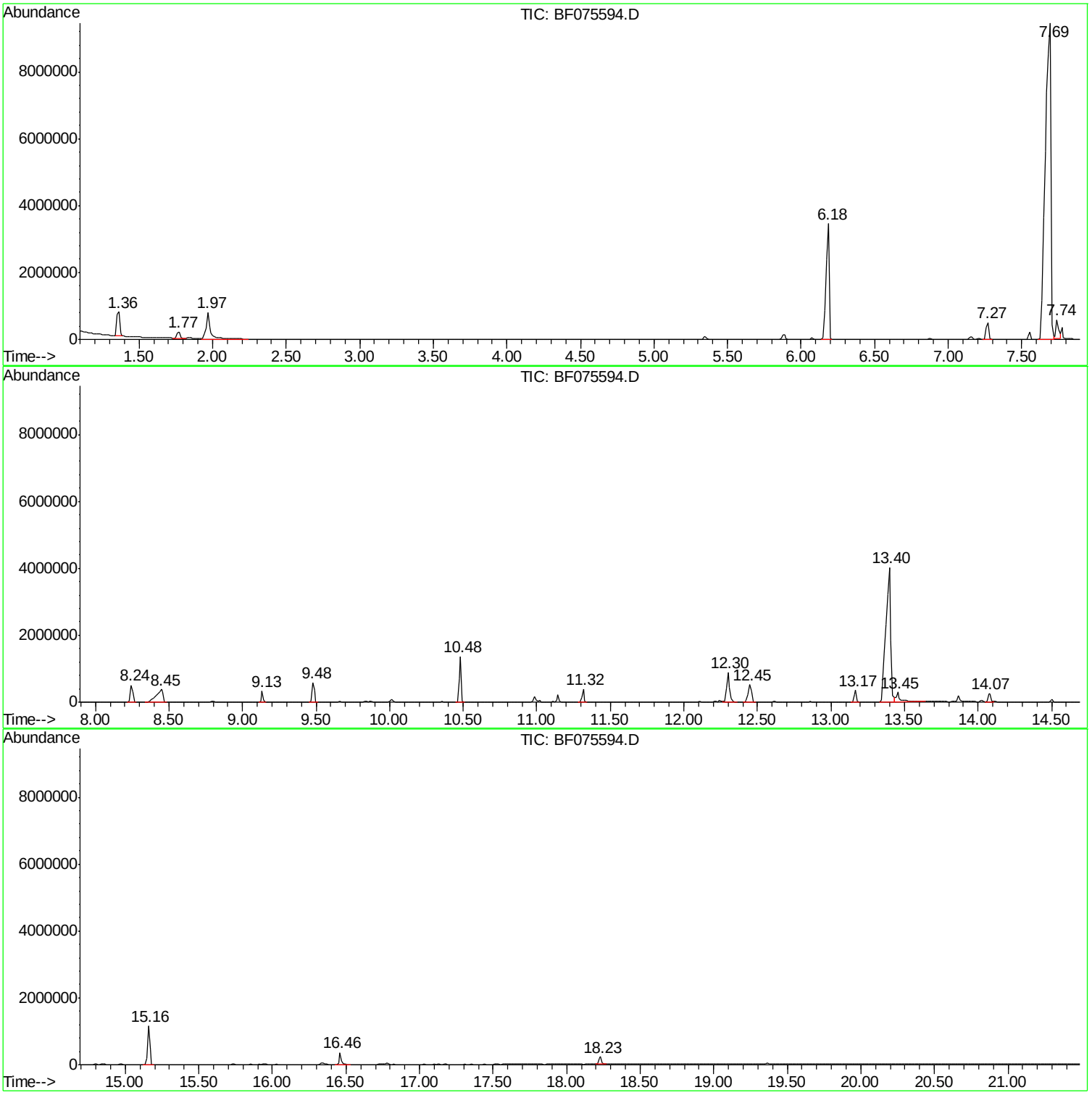
Instrument :
BNA_F
ClientSampleId :
DCW-WW-021-111214

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF075594.D
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Sample : F4742-02
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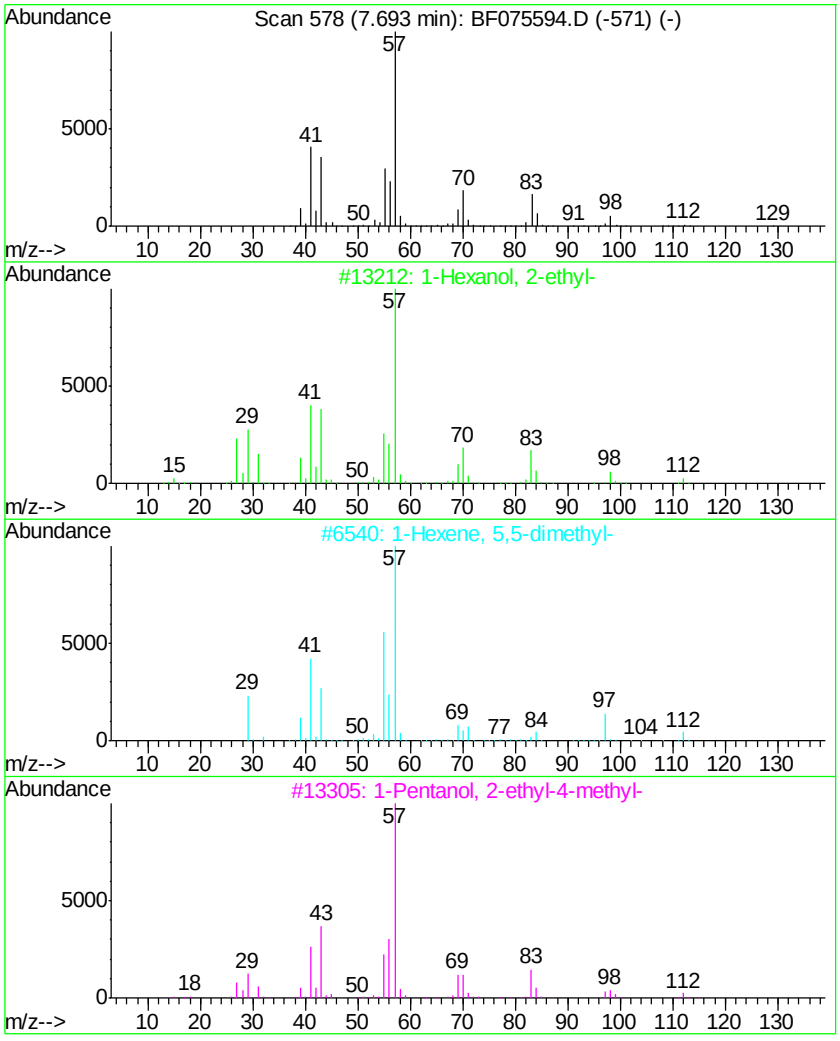
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

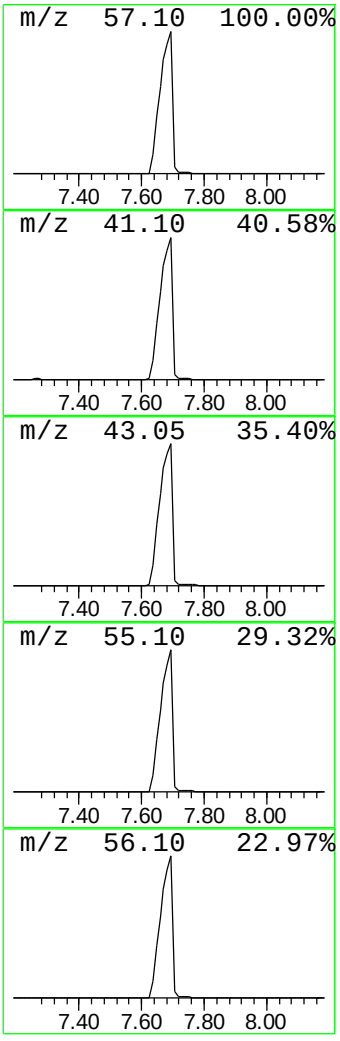
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	20.00 ng	24939000	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	53
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	45
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	42





Library Search Compound Report

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Data File : BF075594.D
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Sample : F4742-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DCW-WW-021-111214

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

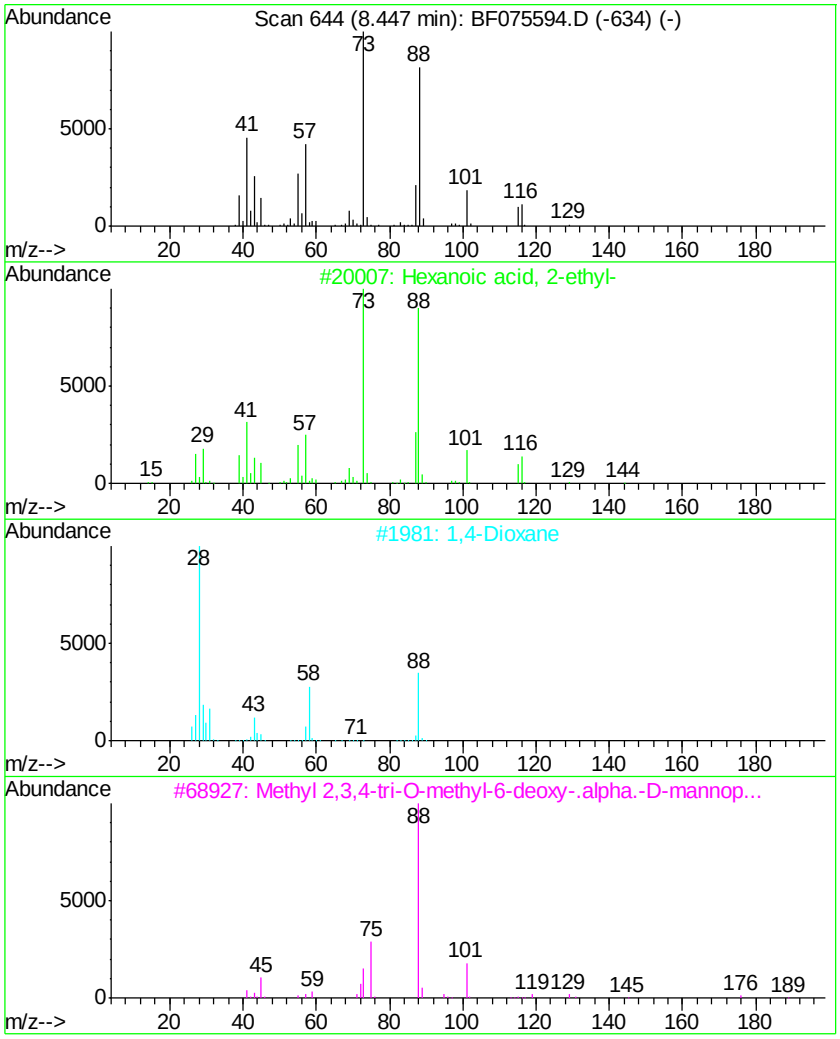
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

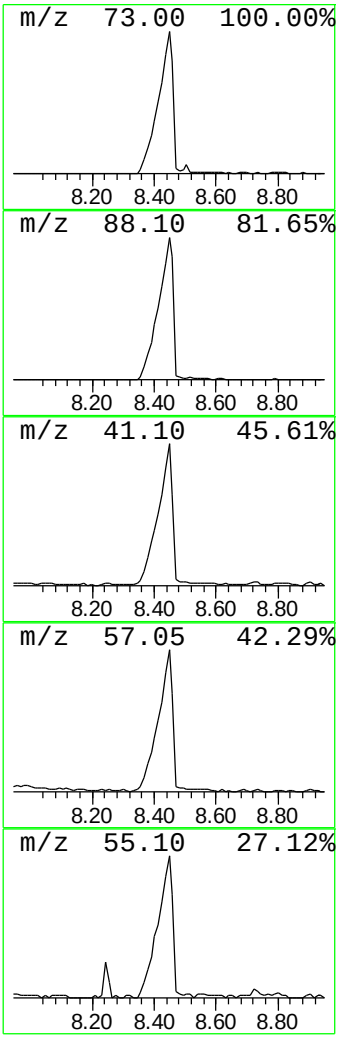
****

Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	91.18 ng	1235890	Naphthalene-d8	9.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	1,4-Dioxane	88	C4H8O2	000123-91-1	47
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
4	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	38
5	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	38





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Data File : BF075594.D
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Operator : TP / JJ
Sample : F4742-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DCW-WW-021-111214

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

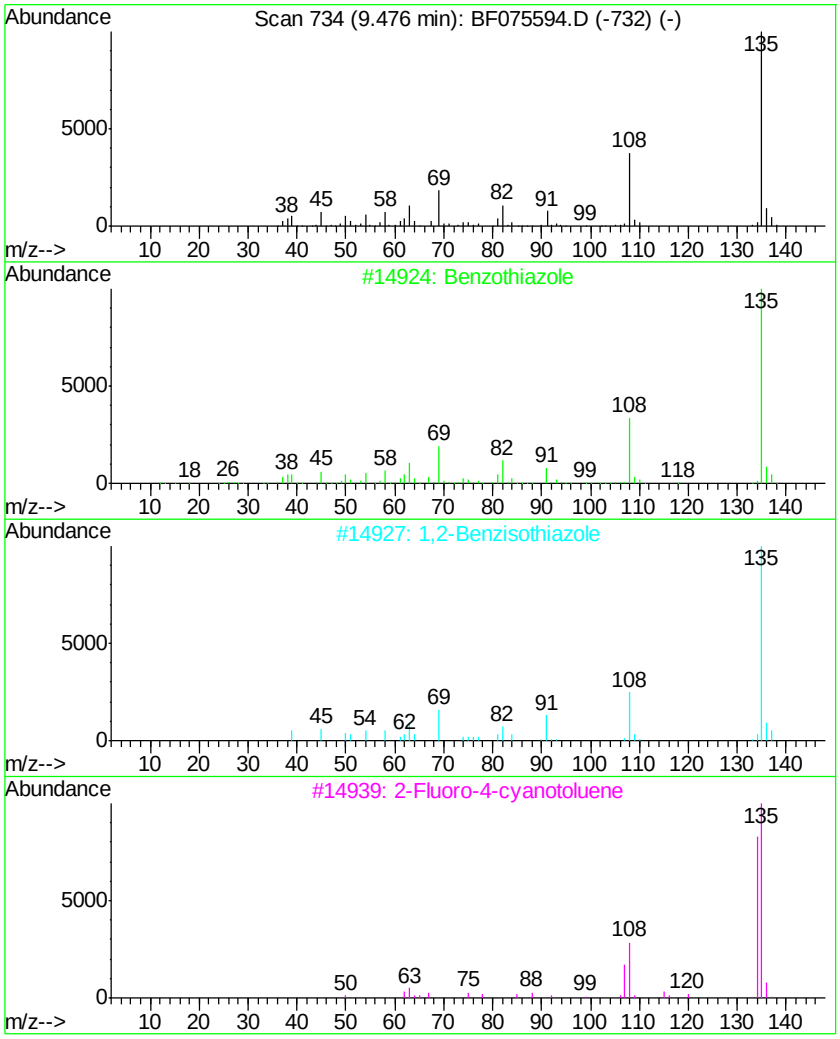
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

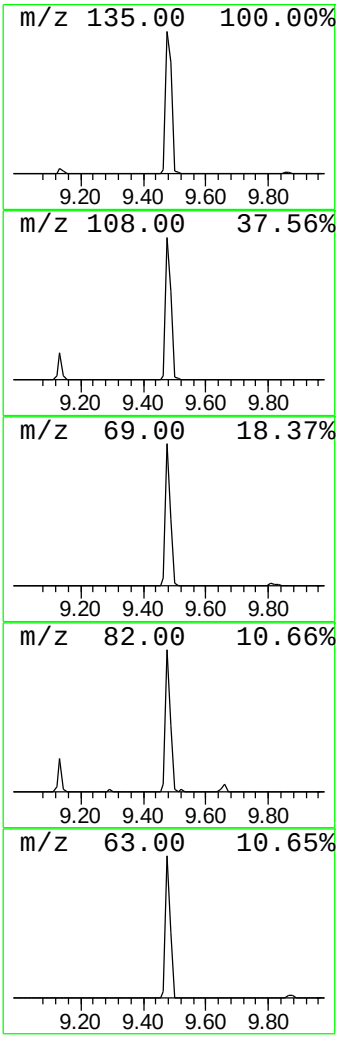
****

Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	49.63 ng	672742	Naphthalene-d8	9.13

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	2-Fluoro-4-cvanotoluene	135	C8H6FN	170572-49-3	64
4	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	58
5	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	56





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Sample : F4742-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DCW-WW-021-111214

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

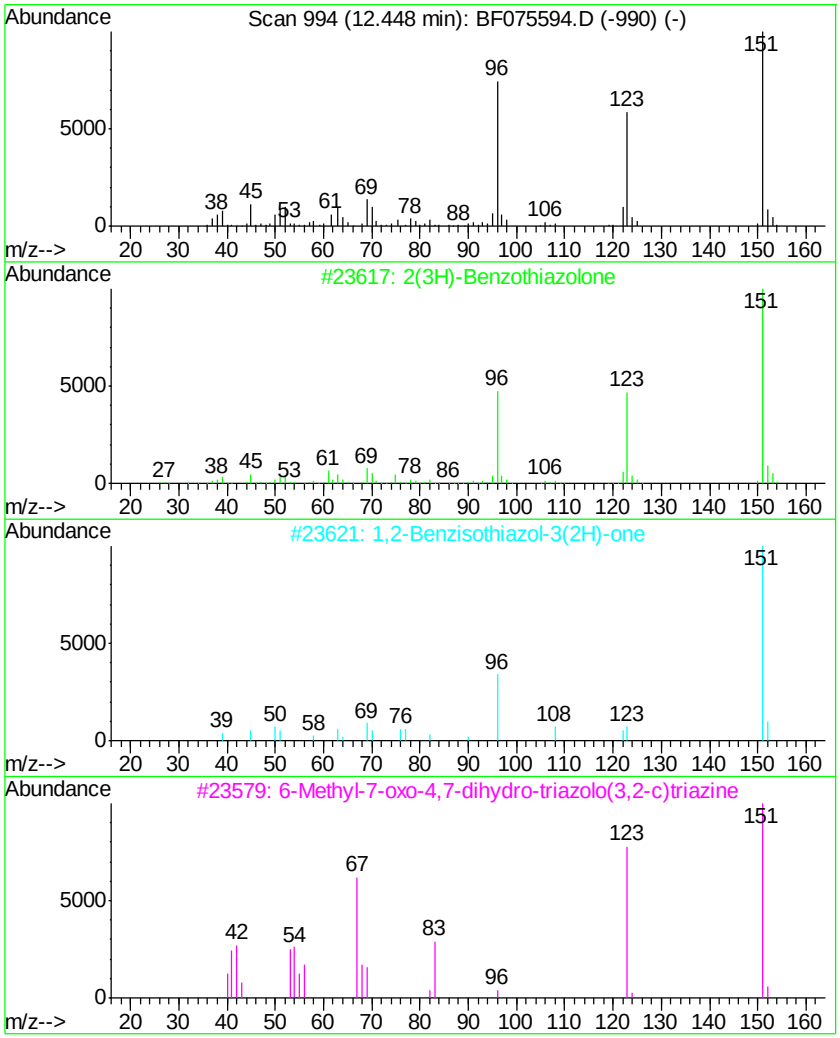
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

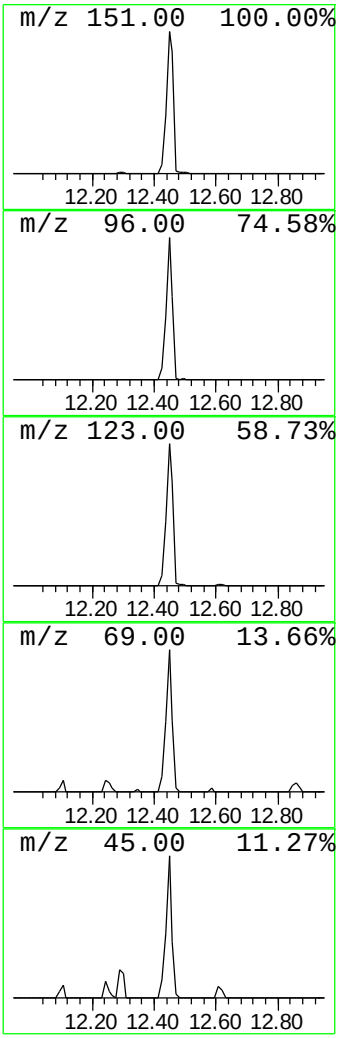
****

Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	40.19 ng	775879	Phenanthrene-d10	13.17

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	50
3	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	43
4	4-Amino-2,1,3-benzothiadiazole	151	C6H5N3S	000767-64-6	27
5	Benzene, fluoro-	96	C6H5F	000462-06-6	27





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Instrument : BNA_F
ClientSampleId : DCW-WW-021-111214

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

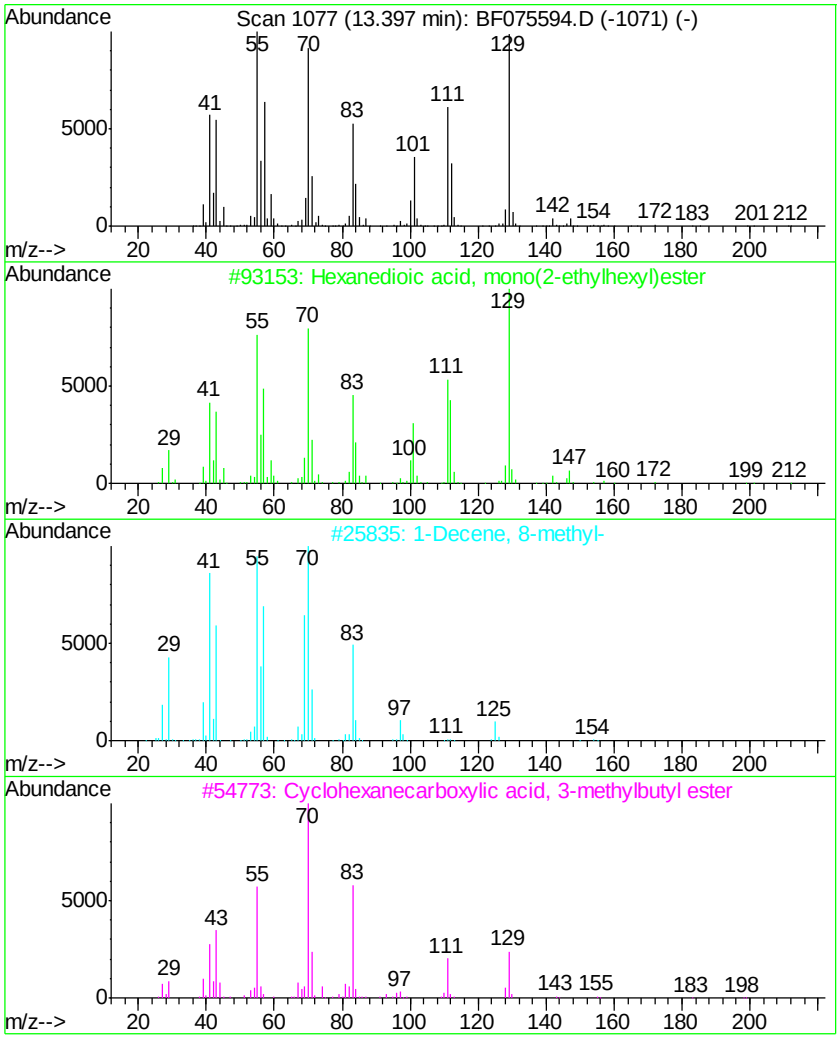
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

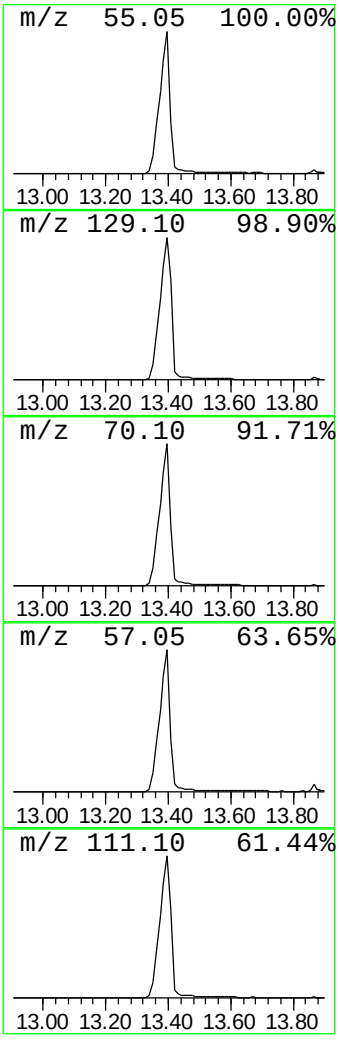
****

Peak Number 6 Hexanedioic acid, mono(2-et... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	488.98 ng	9440430	Phenanthrene-d10	13.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	91
2	1-Decene, 8-methyl-	154	C11H22	061142-79-8	38
3	Cyclohexanecarboxylic acid, 3-me...	198	C12H22O2	025183-19-1	38
4	5-Ethyl-1-nonene	154	C11H22	019780-74-6	35
5	5-Chloropentanoic acid, 2-ethylh...	248	C13H25ClO2	1000293-48-9	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

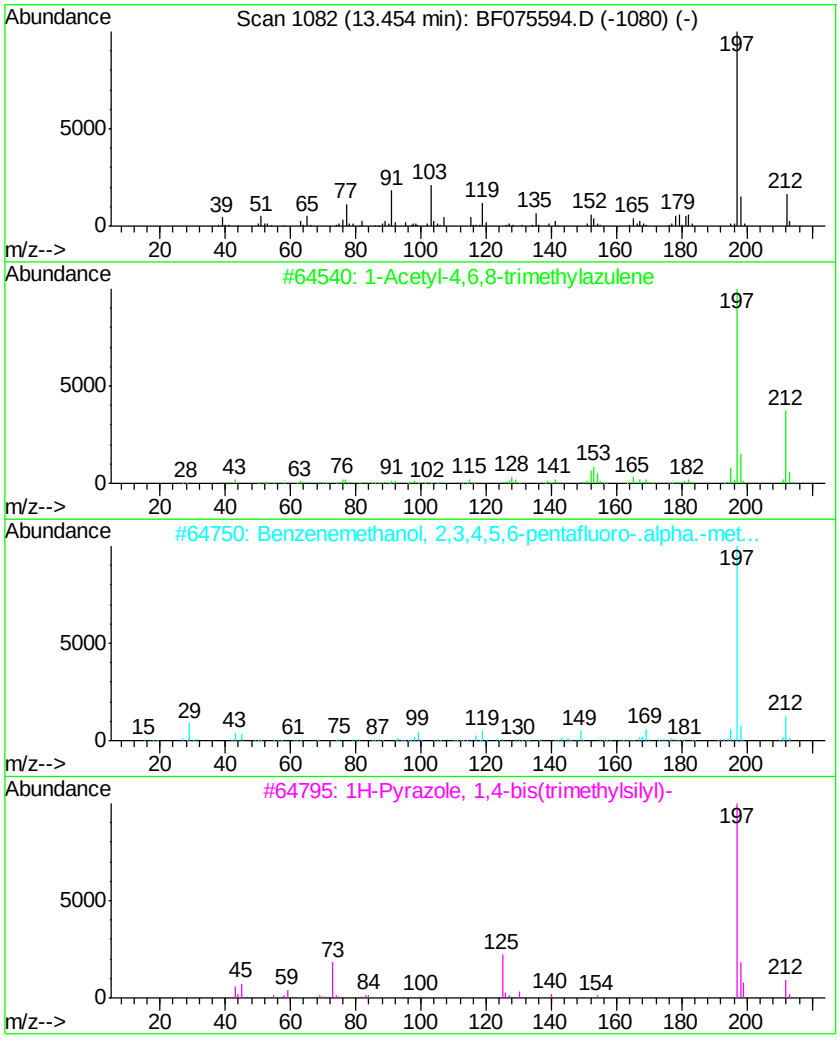
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

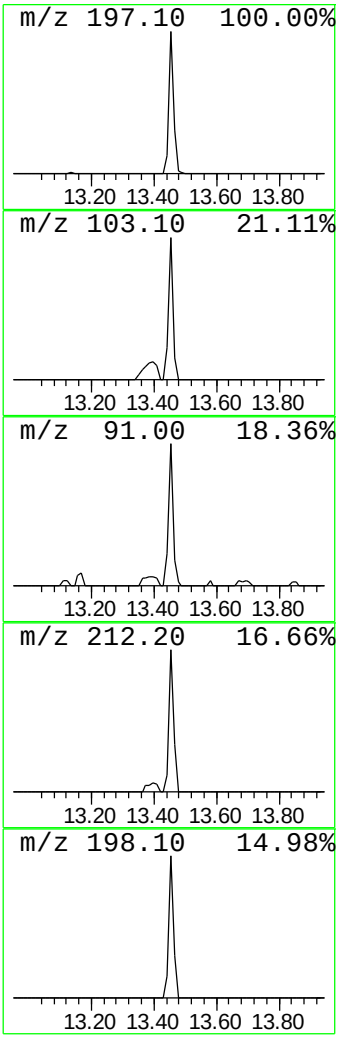
****

Peak Number 7 1-Acetyl-4,6,8-trimethylazu... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	28.08 ng	542097	Phenanthrene-d10	13.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Acetyl-4,6,8-trimethylazulene	212	C15H16O	000834-97-9	52
2	Benzenemethanol, 2,3,4,5,6-penta...	212	C8H5F5O	075853-08-6	50
3	1H-Pyrazole, 1,4-bis(trimethylsi...	212	C9H20N2Si2	052805-95-5	50
4	Benzo[d,e]isocoumarin, 3,3-dimet...	212	C14H12O2	005723-17-1	50
5	4-Hydrazono-5-hydroxyimino-4,5,6...	197	C6H7N5O3	303194-86-7	49





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

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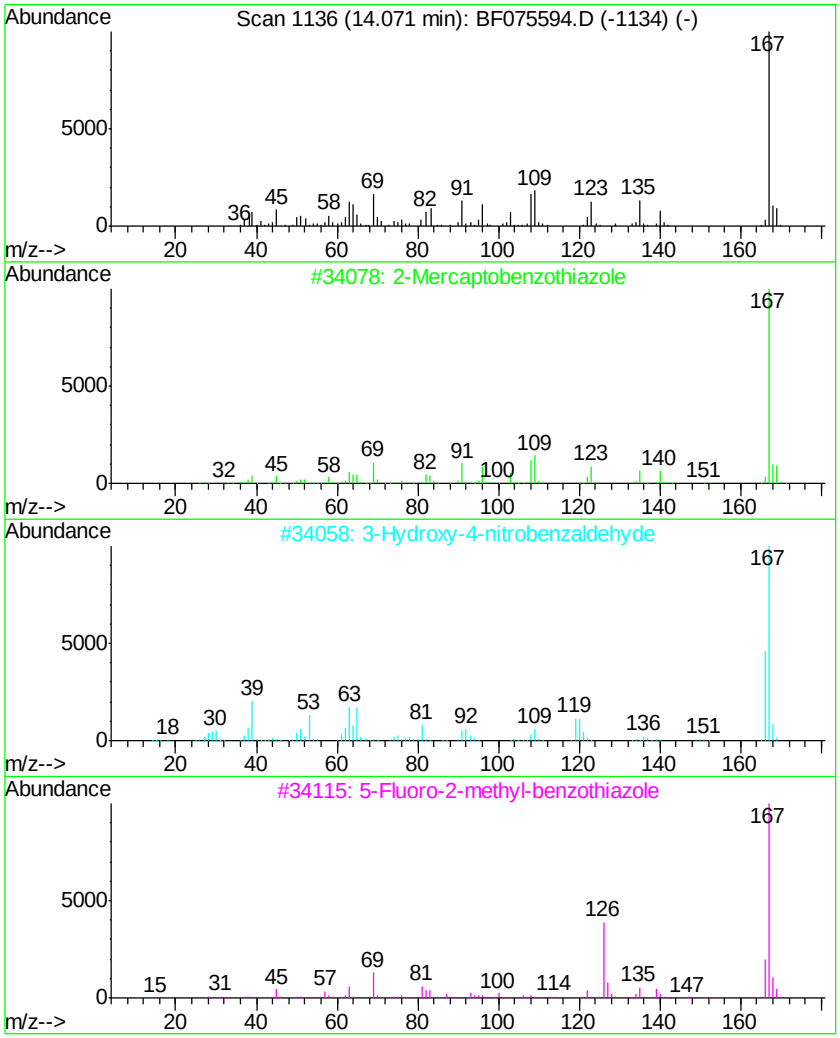
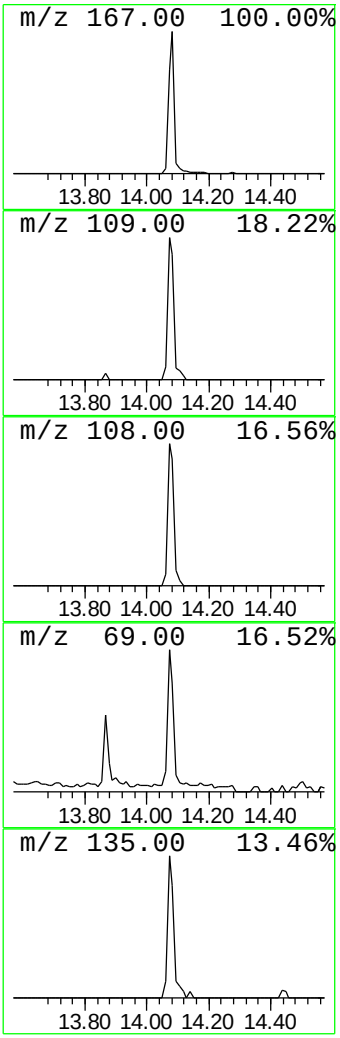
Peak Number 8 2-Mercaptobenzothiazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	19.29 ng	372388	Phenanthrene-d10	13.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
2	3-Hydroxy-4-nitrobenzaldehyde	167	C7H5NO4	000704-13-2	47
3	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	47
4	Benzoxazole, 5-chloro-2-methyl-	167	C8H6ClNO	019219-99-9	43
5	6H-Purine-6-thione, 9-amino-1,9-...	167	C5H5N5S	020914-56-1	43





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-ethyl-	7.69	20.0	ng	24939000	1	7.56	24939000	20.0
Hexanoic acid, 2-...	8.45	91.2	ng	1235890	2	9.13	271098	20.0
Benzothiazole	9.48	49.6	ng	672742	2	9.13	271098	20.0
2(3H)-Benzothiazo...	12.45	40.2	ng	775879	4	13.17	386131	20.0
Hexanedioic acid,...	13.40	489.0	ng	9440430	4	13.17	386131	20.0
1-Acetyl-4,6,8-tr...	13.45	28.1	ng	542097	4	13.17	386131	20.0
2-Mercaptobenzoth...	14.07	19.3	ng	372388	4	13.17	386131	20.0