LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075595.D
Acq On : 16 Nov 2014 22:33
Operator : TP / JJ
Sample : F4742-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DCW-WW-021A-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	585907	744576	2.76%	1.509%
2	1.967	73	77	94	rVB2	619559	1123436	4.17%	2.277%
3	6.185	442	446	448	rBV	2814230	3800799	14.11%	7.703%
4	7.270	538	541	543	rVB	434401	553991	2.06%	1.123%
5	7.693	571	578	580	rBV	8614775	26933789	100.00%	54.584%
6	7.739	580	582	584	rVV	523688	603837	2.24%	1.224%
7	7.773	584	585	587	rVB	390180	283715	1.05%	0.575%
8	8.242	624	626	629	rBV	416063	525227	1.95%	1.064%
9	8.459	635	645	648	rBV	349966	1191577	4.42%	2.415%
10	9.476	732	734	737	rBV	525025	598380	2.22%	1.213%
11	10.482	819	822	824	rBV	1109441	1141653	4.24%	2.314%
12	11.316	892	895	897	rBV	265823	273008	1.01%	0.553%
13	12.299	978	981	986	rVB2	662889	978026	3.63%	1.982%
14	12.448	991	994	997	rBV	369825	620239	2.30%	1.257%
15	13.168	1054	1057	1059	rVB	227618	277257	1.03%	0.562%
16	13.397	1070	1077	1080	rBV	2817990	7683779	28.53%	15.572%
17	13.454	1080	1082	1091	rVB	202170	311357	1.16%	0.631%
18	15.157	1228	1231	1233	rBV	1098346	1080912	4.01%	2.191%
19	16.460	1342	1345	1347	rBV	241178	315983	1.17%	0.640%
20	18.197	1494	1497	1500	rBV	213971	302053	1.12%	0.612%

Sum of corrected areas: 49343594

LSC Report - Integrated Chromatogram

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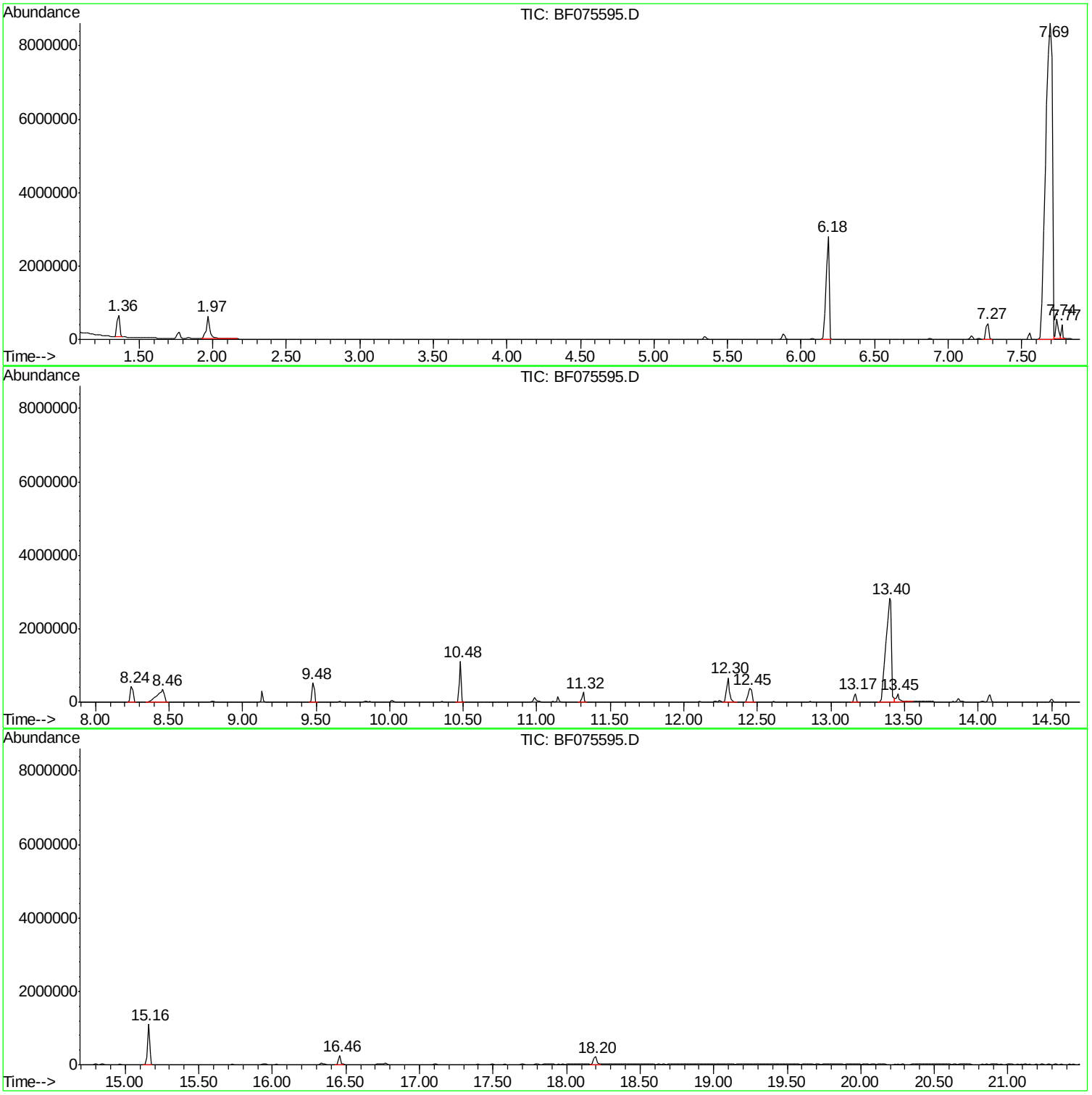
Sample : F4742-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075595.D
Acq On : 16 Nov 2014 22:33
Operator : TP / JJ
Sample : F4742-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

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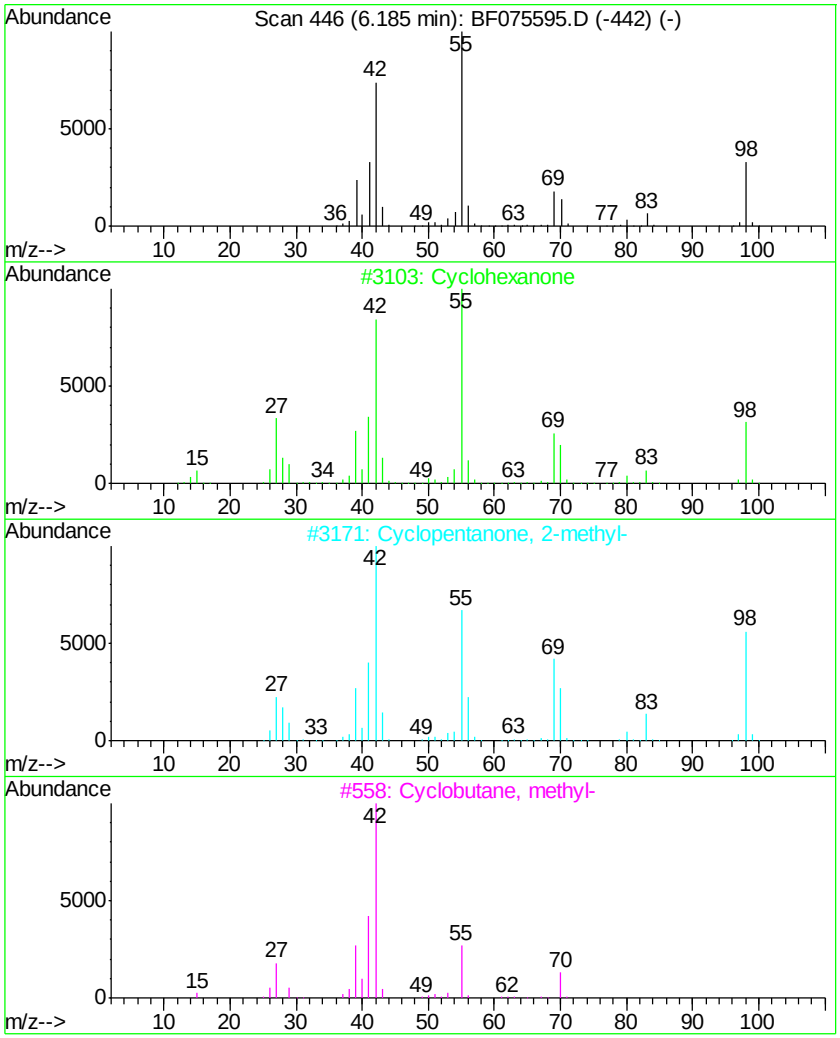
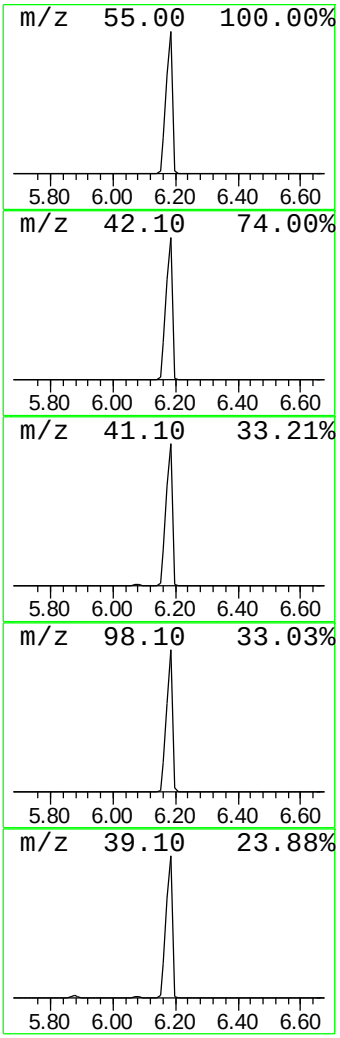
Peak Number 1 Cyclohexanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	2.82 ng	3800800	1,4-Dichlorobenzene-d4	7.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	78
2	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	52
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	43
4	2H-Imidazol-2-one, 1,3-dihydro-4...	98	C4H6N2O	001192-34-3	38
5	2-Methyl-3,4,5,6-tetrahydropyrazine	98	C5H10N2	344240-21-7	36





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Data File : BF075595.D
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Operator : TP / JJ
Sample : F4742-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

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

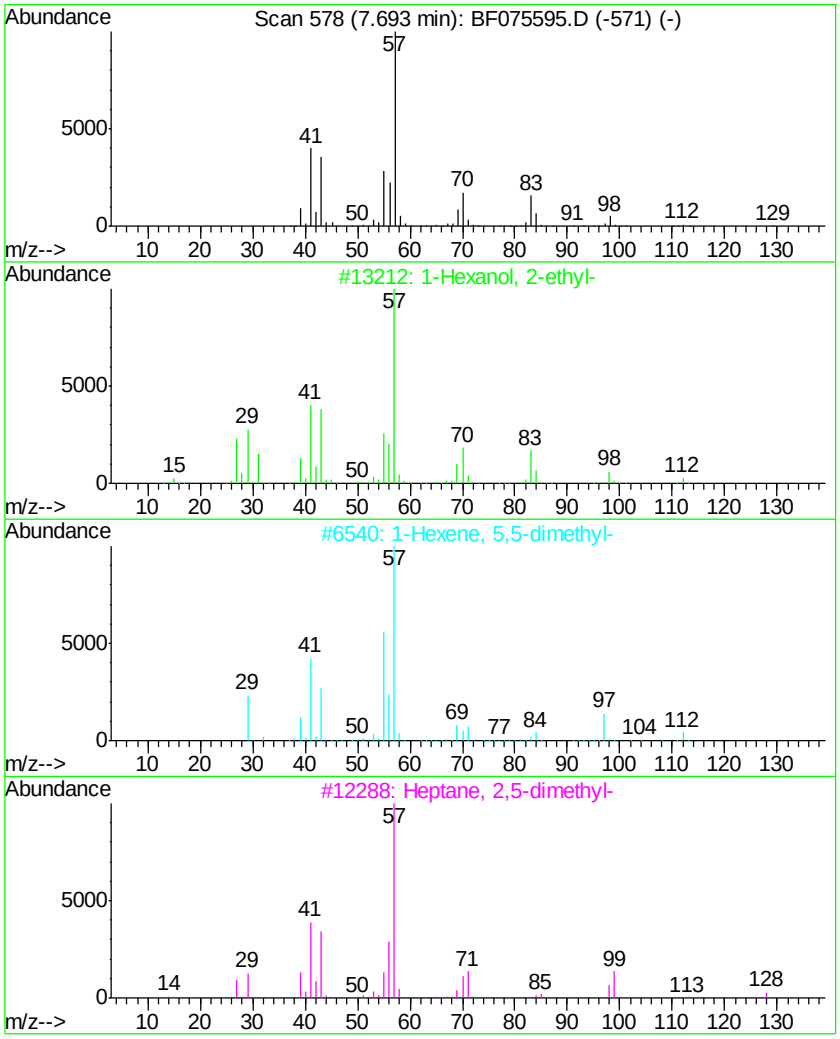
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

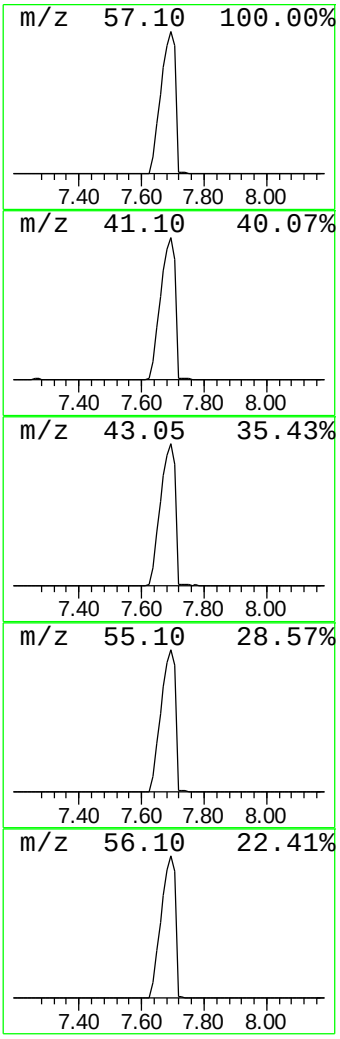
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	20.00 ng	26933800	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	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	45
4	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	42
5	dl-2-Ethylhexyl chloroformate	192	C9H17ClO2	024468-13-1	40





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075595.D
Acq On : 16 Nov 2014 22:33
Operator : TP / JJ
Sample : F4742-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

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

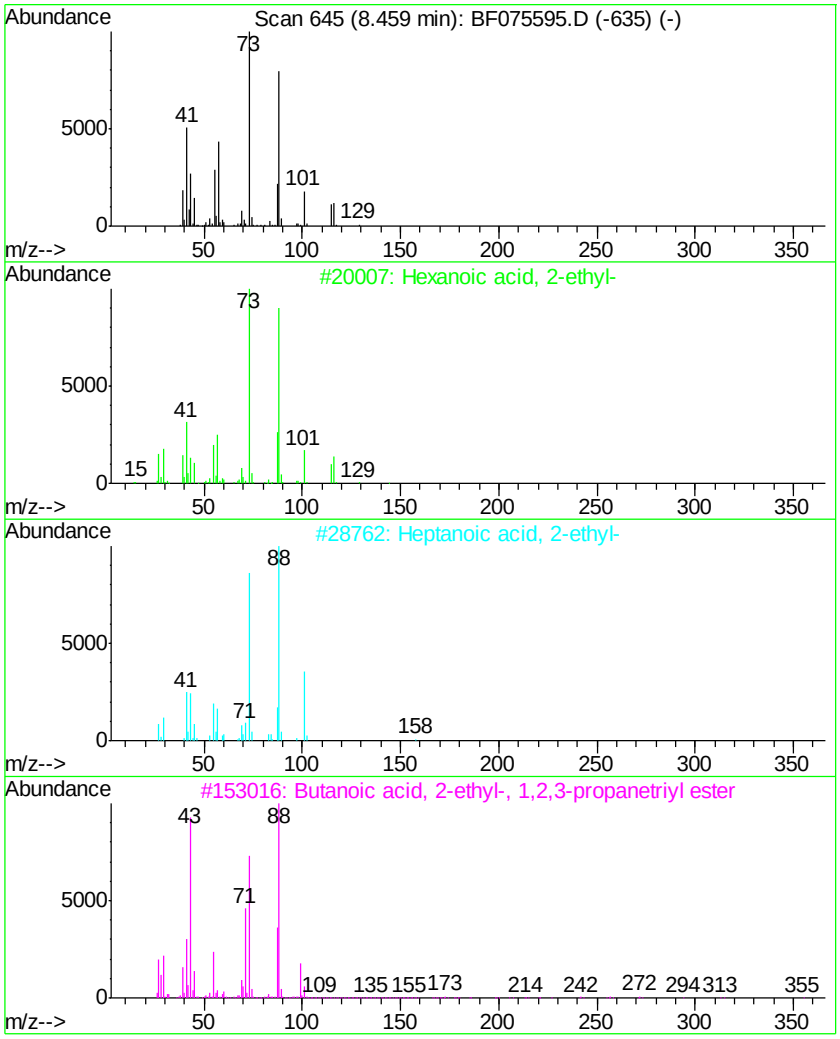
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

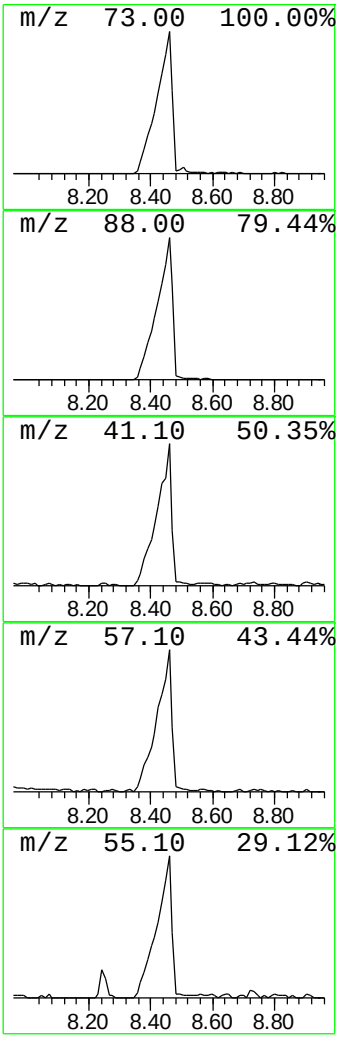
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	39.83 ng	1191580	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	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
4	1,4-Dioxane	88	C4H8O2	000123-91-1	47
5	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40





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Data File : BF075595.D
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Operator : TP / JJ
Sample : F4742-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

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

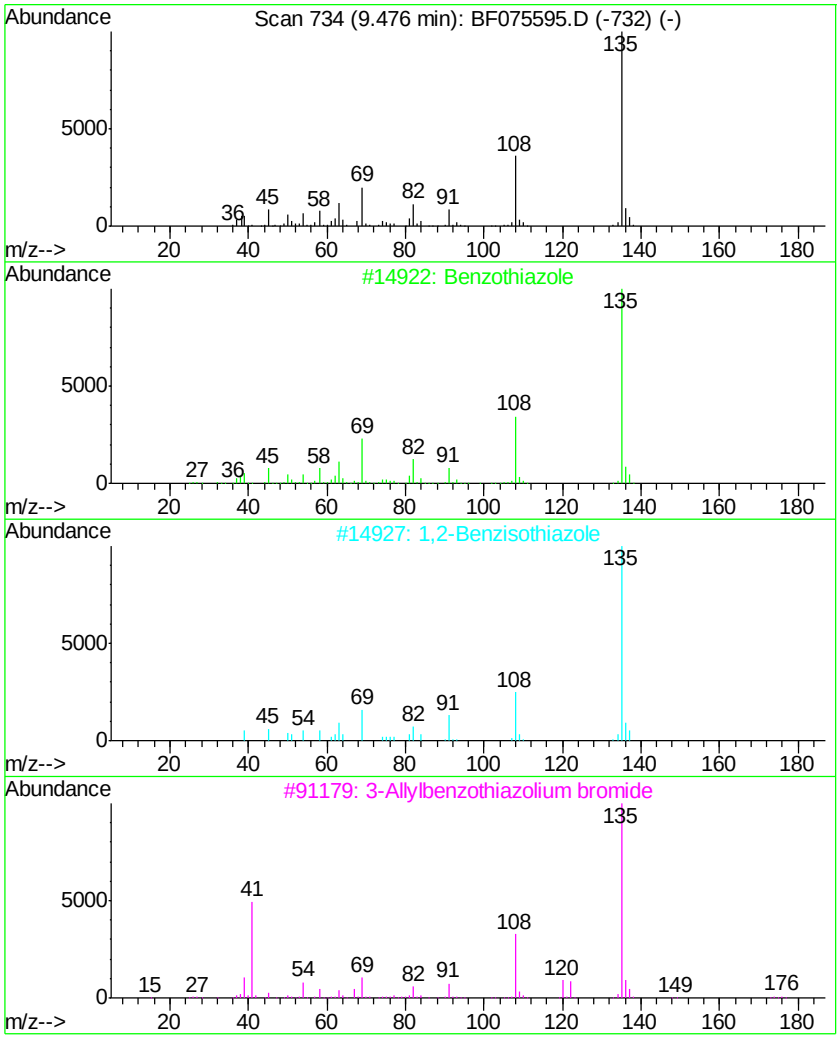
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

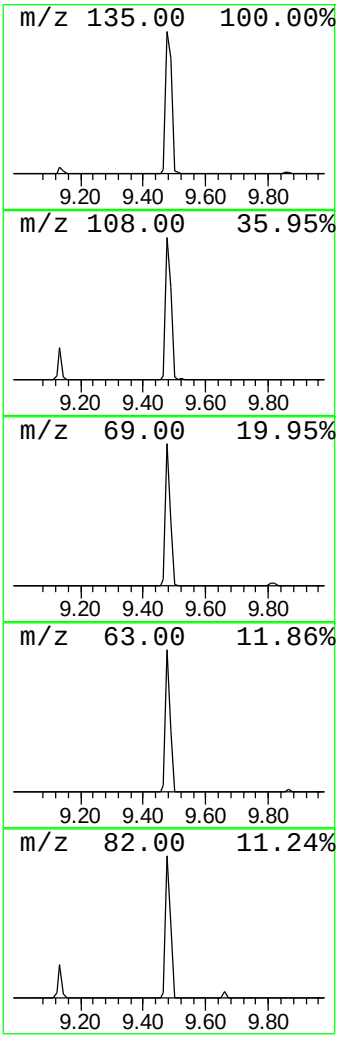
****

Peak Number 4 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	20.00 ng	598380	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	90
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
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\BF111414\
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Sample : F4742-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

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

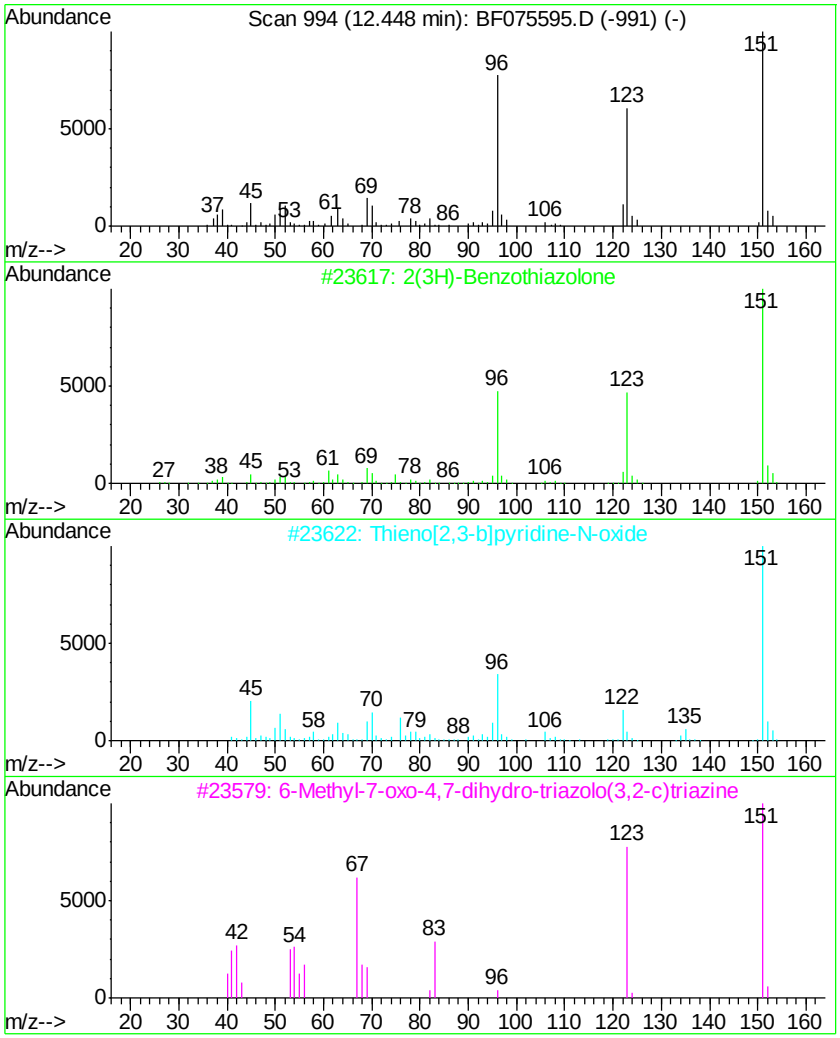
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

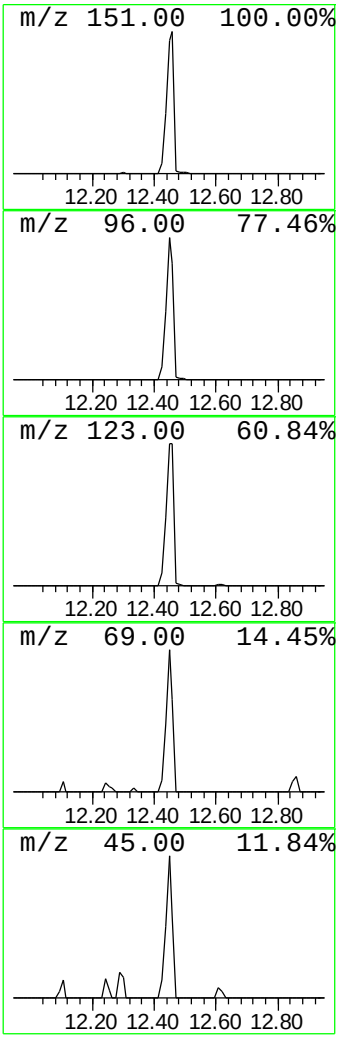
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	44.74 ng	620239	Phenanthrene-d10	13.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
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	38
4	4-Methoxyformanilide	151	C8H9NO2	023896-88-0	35
5	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	35





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

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

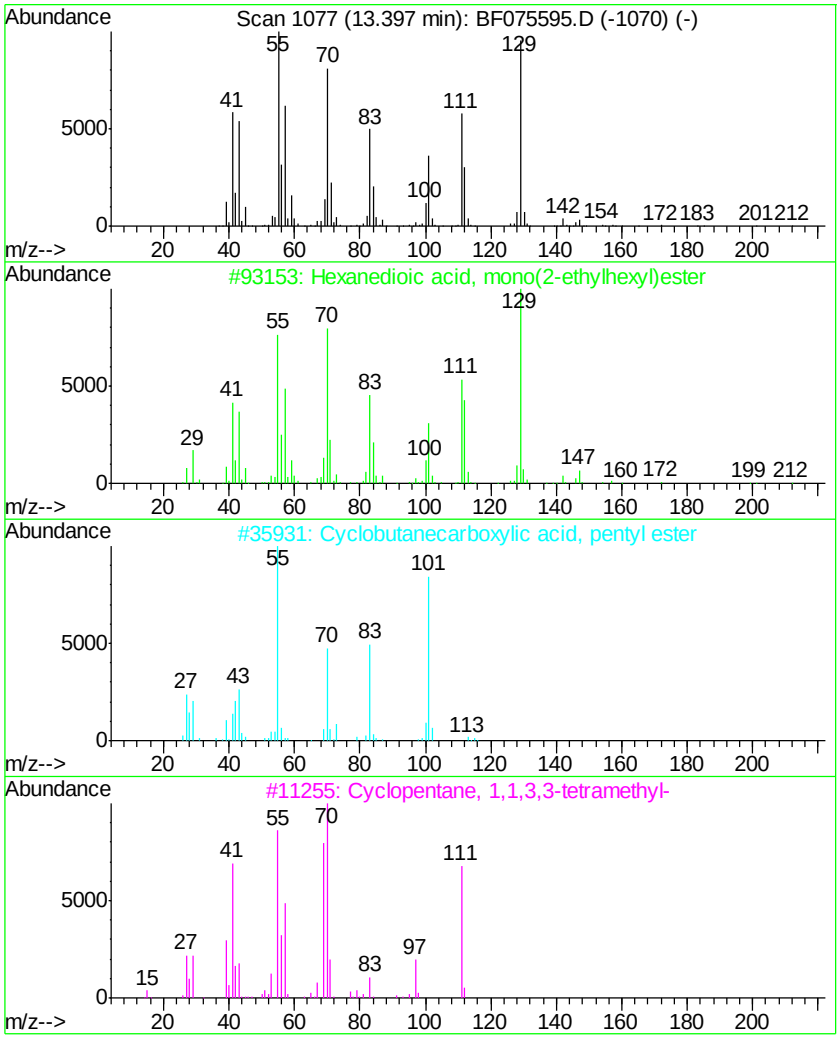
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

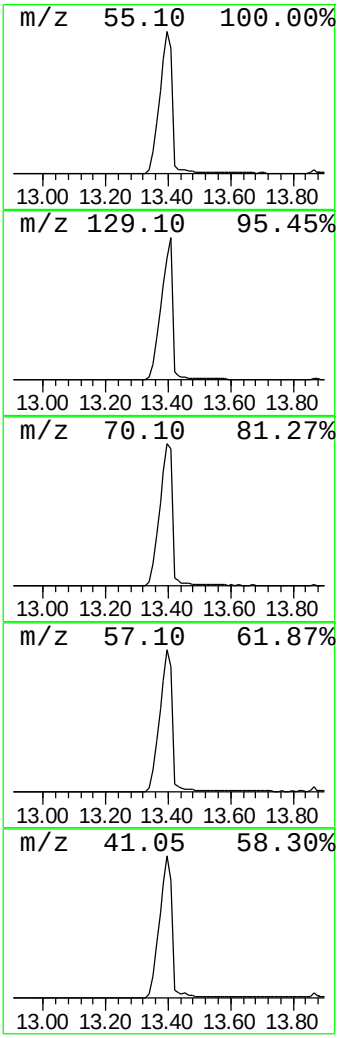
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	554.27 ng	7683780	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	Cyclobutanecarboxylic acid, pent...	170	C10H18O2	1000280-40-2	35
3	Cyclopentane, 1,1,3,3-tetramethyl-	126	C9H18	050876-33-0	35
4	Cyclohexanecarboxylic acid, 3-me...	198	C12H22O2	025183-19-1	35
5	iso-Amyl tiglate	170	C10H18O2	066917-62-2	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

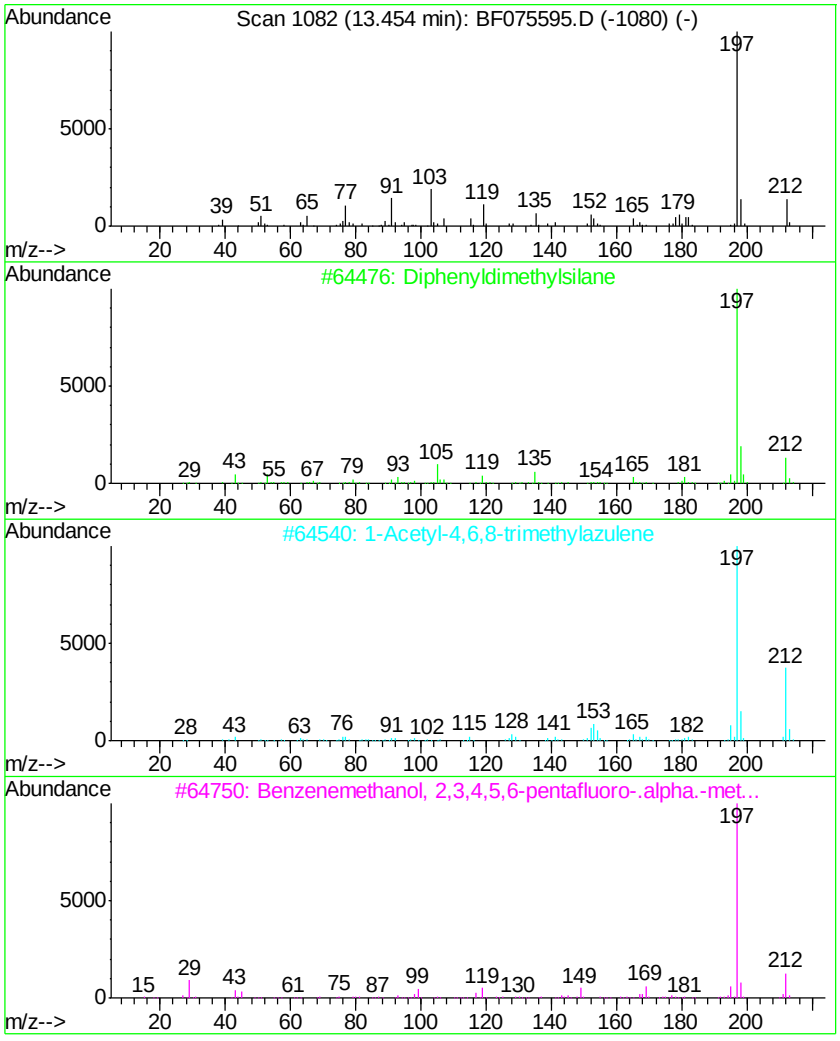
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

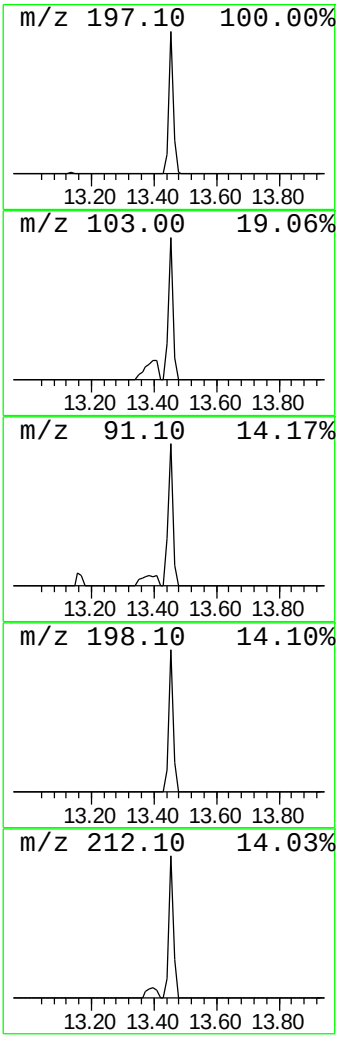
****

Peak Number 7 Diphenyldimethylsilane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	22.46 ng	311357	Phenanthrene-d10	13.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenyldimethylsilane	212	C14H16Si	000778-24-5	62
2	1-Acetyl-4,6,8-trimethylazulene	212	C15H16O	000834-97-9	58
3	Benzenemethanol, 2,3,4,5,6-penta...	212	C8H5F5O	075853-08-6	58
4	1H-Pyrazole, 1,4-bis(trimethylsi...	212	C9H20N2Si2	052805-95-5	50
5	Benzo[d,E]isocoumarin, 3,3-dimet...	212	C14H12O2	005723-17-1	50





Tentatively Identified Compound (LSC) summary

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Acq On : 16 Nov 2014 22:33
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexanone	6.18	2.8	ng	3800800	1	7.56	26933800	20.0
1-Hexanol, 2-ethyl-	7.69	20.0	ng	26933800	1	7.56	26933800	20.0
Hexanoic acid, 2-...	8.46	39.8	ng	1191580	2	9.13	598380	20.0
Benzothiazole	9.48	20.0	ng	598380	2	9.13	598380	20.0
2(3H)-Benzothiazo...	12.45	44.7	ng	620239	4	13.17	277257	20.0
Hexanedioic acid,...	13.40	554.3	ng	7683780	4	13.17	277257	20.0
Diphenyldimethyls...	13.45	22.5	ng	311357	4	13.17	277257	20.0