LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
Data File : BF098207.D
Acq On : 31 Aug 2017 21:08
Operator : SJ/JU
Sample : I4963-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3833-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-BF081517.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	4.910	476	480	489	rBV	78800	105062	2.80%	0.389%
2	5.322	543	550	564	rBV	2145319	2161313	57.56%	8.006%
3	6.357	721	726	729	rBV	1781653	1601877	42.66%	5.934%
4	6.486	743	748	752	rBV	2862324	3090385	82.31%	11.447%
5	6.716	783	787	791	rBV	936797	760149	20.25%	2.816%
6	6.875	809	814	817	rBV	2659671	2398161	63.87%	8.883%
7	6.904	817	819	824	rVB	63507	56826	1.51%	0.210%
8	7.286	878	884	887	rBV	2132741	2150776	57.28%	7.967%
9	7.792	967	970	975	rBV4	35458	41674	1.11%	0.154%
10	7.998	1001	1005	1009	rBV	1140361	1012027	26.95%	3.749%
11	8.280	1049	1053	1058	rBV	700528	605956	16.14%	2.245%
12	9.080	1183	1189	1192	rBV	3792092	3754657	100.00%	13.908%
13	9.186	1203	1207	1214	rVB5	23923	41983	1.12%	0.156%
14	9.751	1299	1303	1307	rBV2	1273997	1121413	29.87%	4.154%
15	10.380	1406	1410	1414	rBV	38813	38994	1.04%	0.144%
16	10.545	1432	1438	1441	rBV	2115108	2173442	57.89%	8.051%
17	10.657	1453	1457	1466	rVB	297357	333157	8.87%	1.234%
18	11.233	1551	1555	1562	rVB	1256320	1082321	28.83%	4.009%
19	11.957	1675	1678	1686	rBV	96110	112868	3.01%	0.418%
20	12.821	1820	1825	1829	rBV	2739373	2965862	78.99%	10.986%
21	13.868	1999	2003	2007	rBV	782986	694552	18.50%	2.573%
22	15.286	2240	2244	2254	rVB	530282	692945	18.46%	2.567%

Sum of corrected areas: 26996400

LSC Report - Integrated Chromatogram

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Misc :
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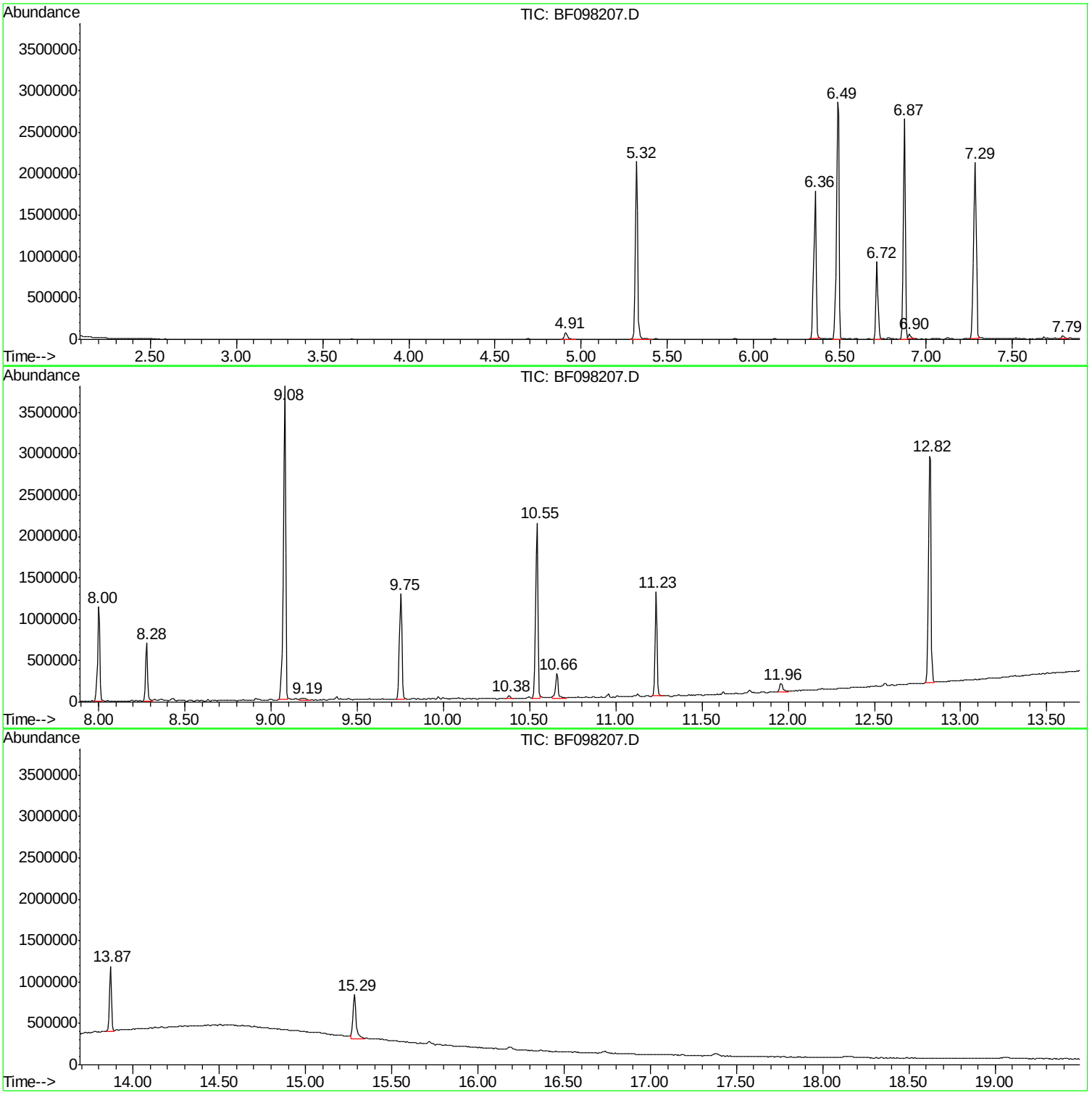
Instrument : BNA_F
ClientSampleId : 3833-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
Data File : BF098207.D
Acq On : 31 Aug 2017 21:08
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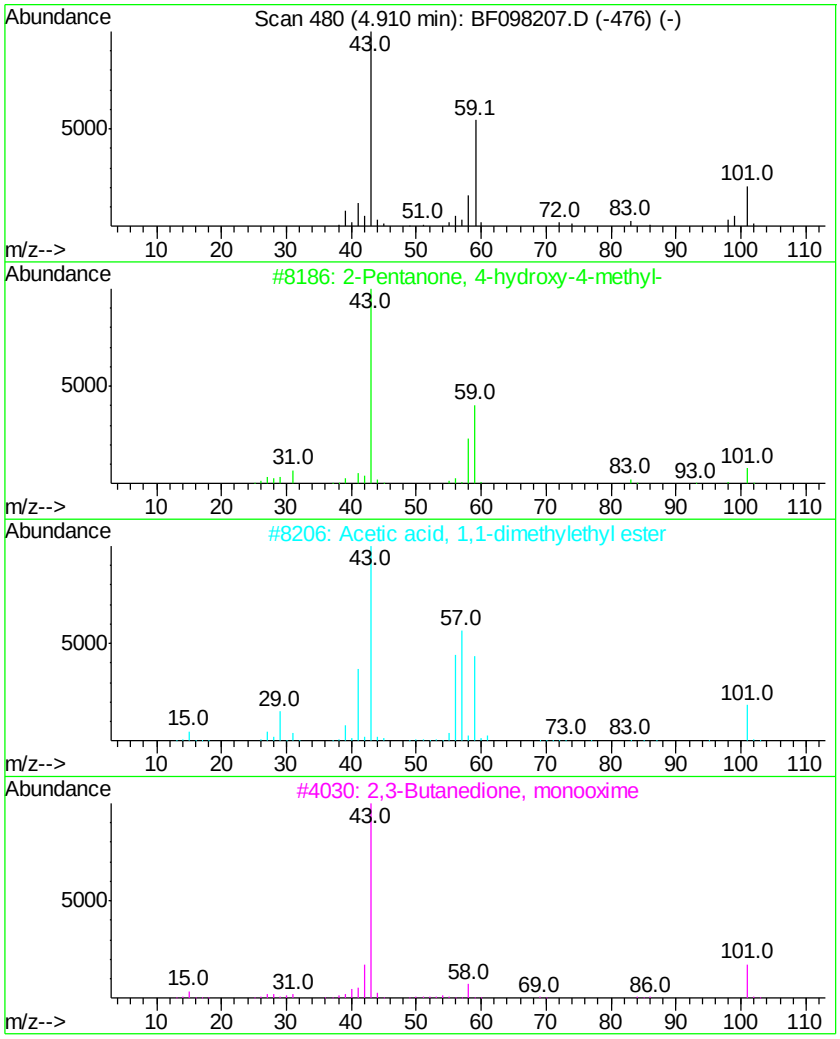
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

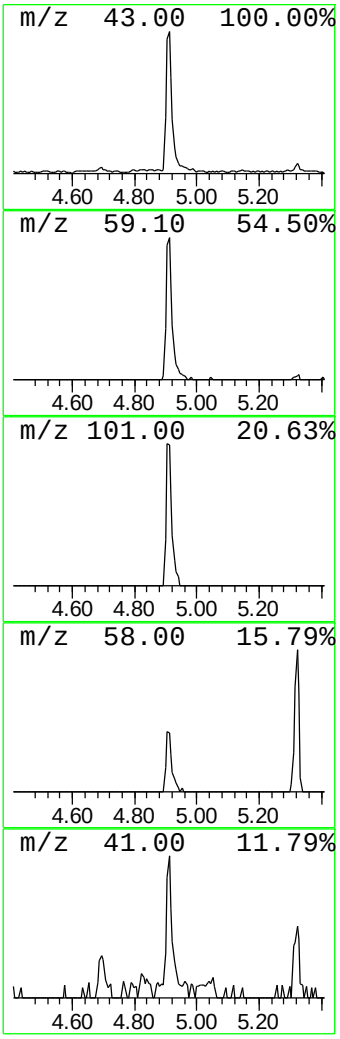
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.76 ng	105062	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	25





Library Search Compound Report

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3833-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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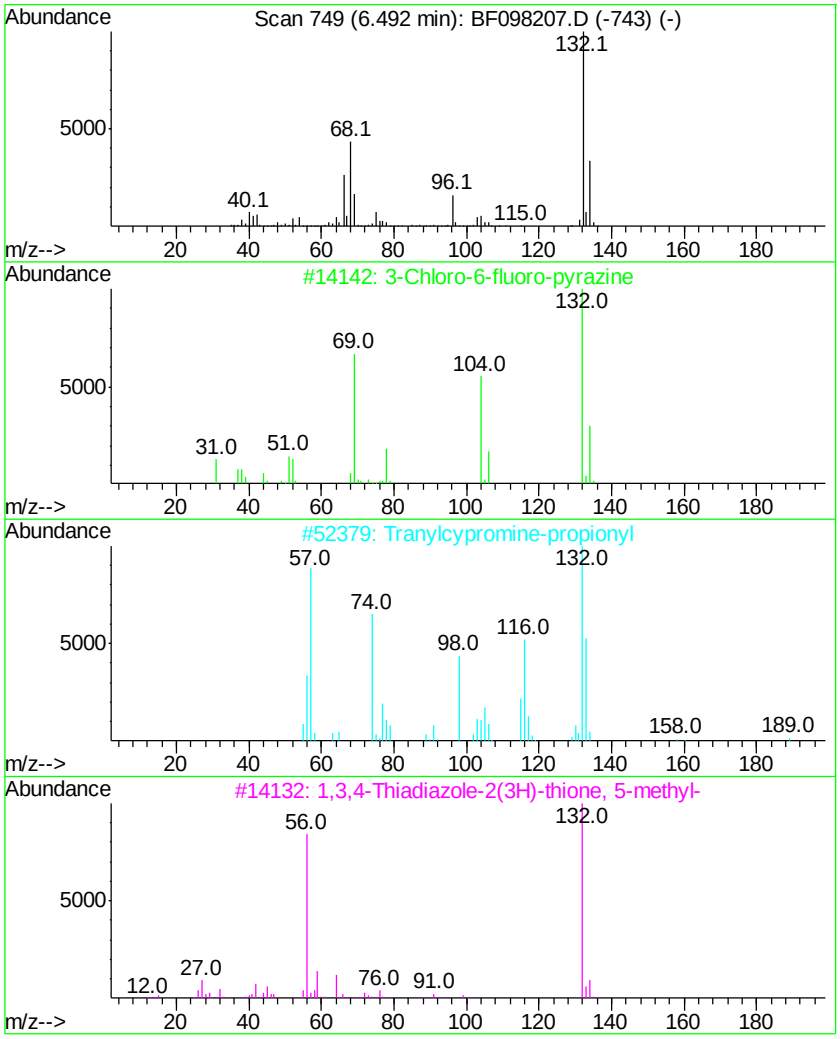
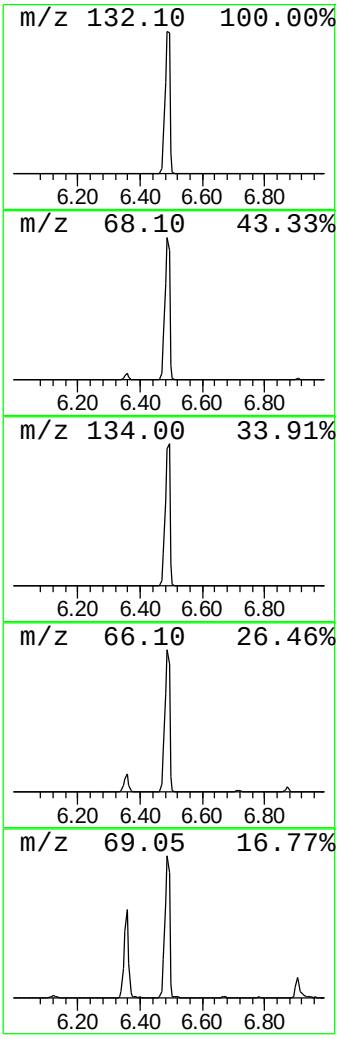
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	81.31 ng	3090390	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : SJ/JU
Sample : I4963-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3833-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

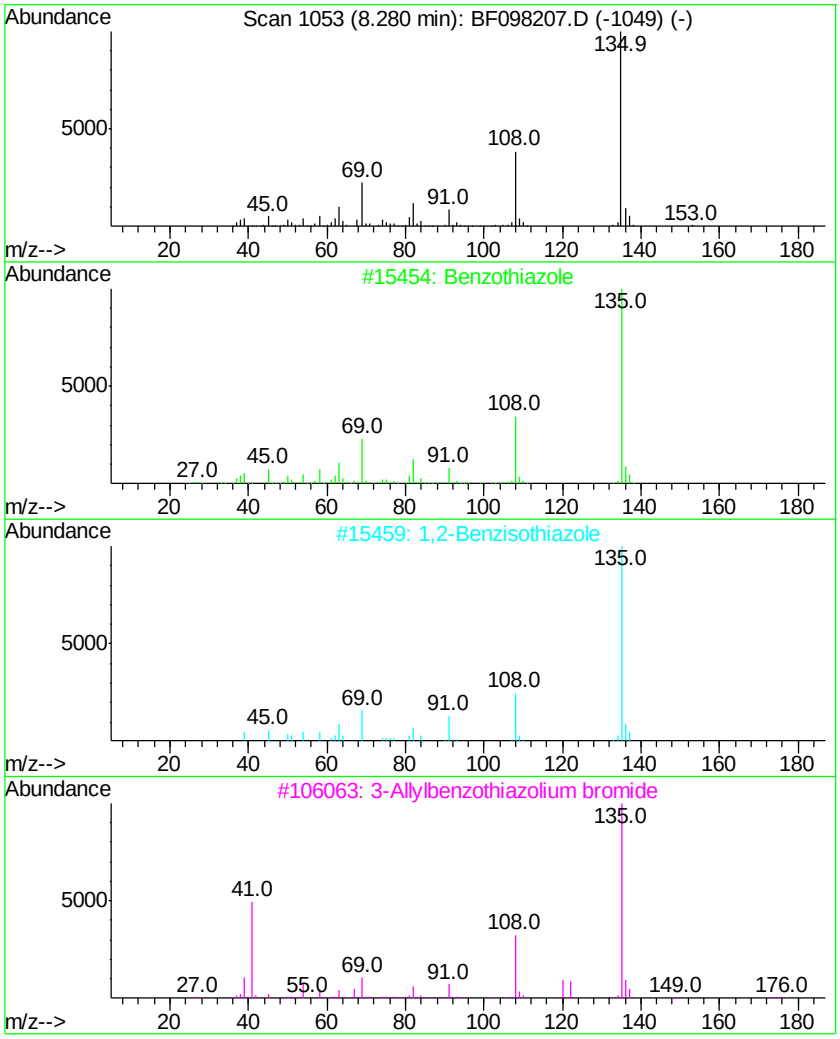
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

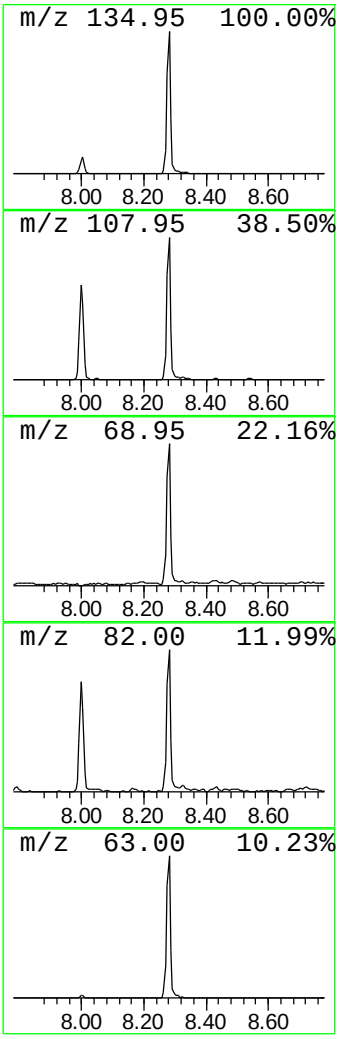
****

Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	11.98 ng	605956	Naphthalene-d8	8.00

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	72
5	2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	72





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Data File : BF098207.D
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Operator : SJ/JU
Sample : I4963-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3833-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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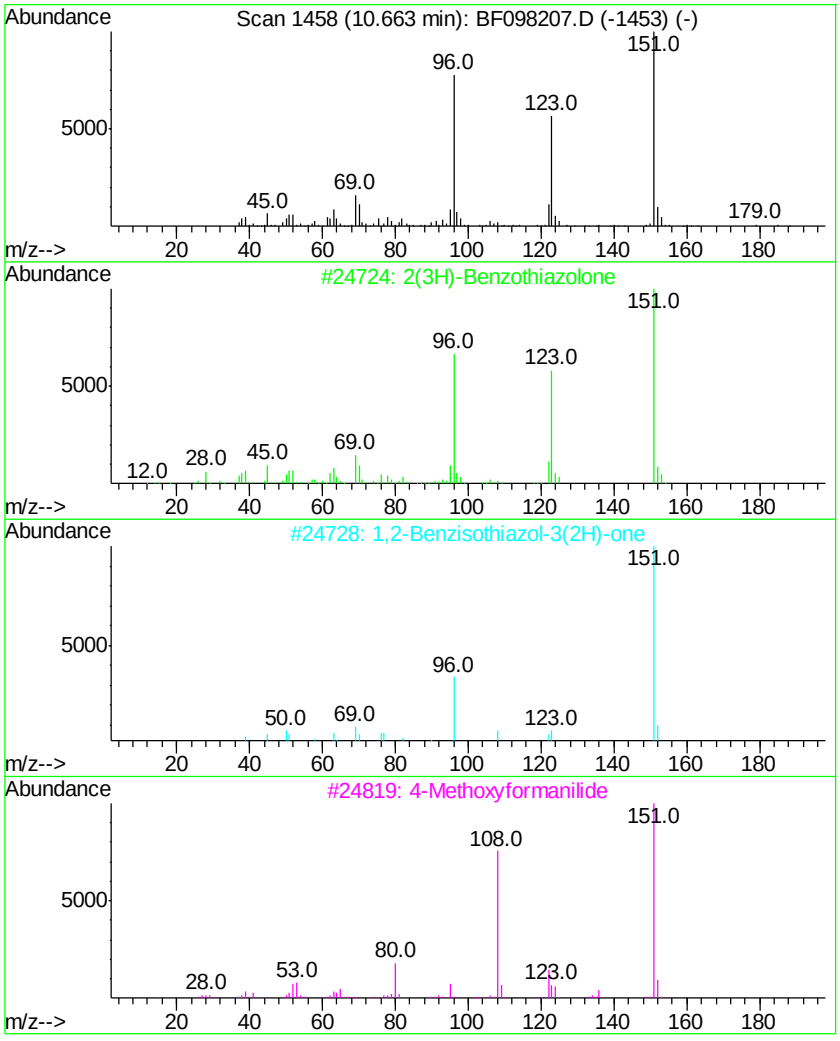
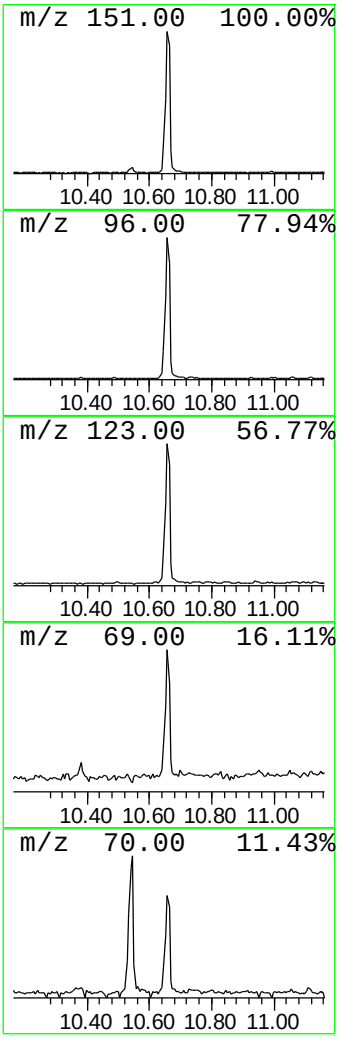
Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	6.16 ng	333157	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	95
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	59
3	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	38
4	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	32
5	1,2,4-Triazolo[4,3-a]pyridine-3(...	151	C6H5N3S	006952-68-7	27





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Sample : I4963-14
Misc :
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Instrument : BNA_F
ClientSampleId : 3833-PA4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
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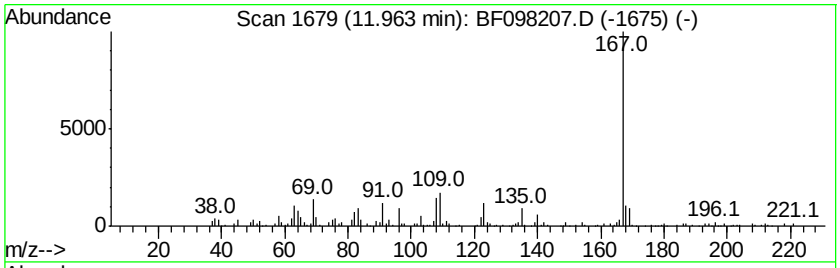
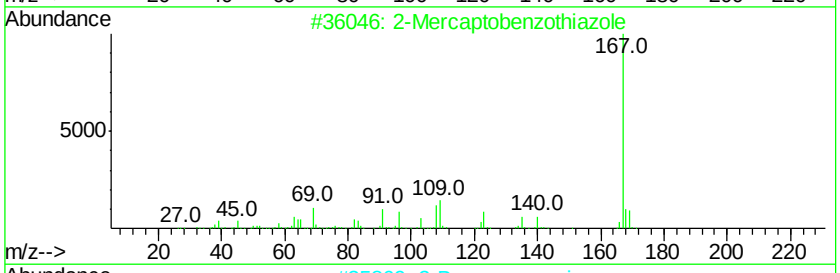
****

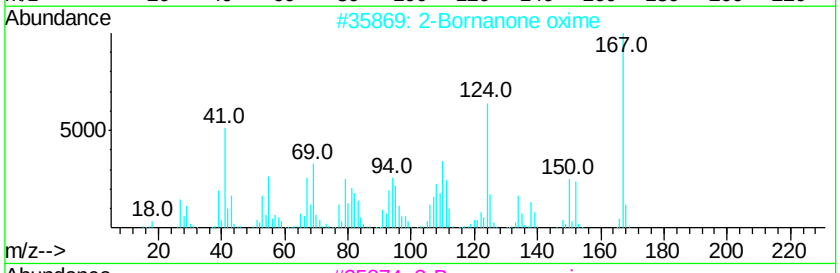
Peak Number 6 2-Mercaptobenzothiazole Concentration Rank 6

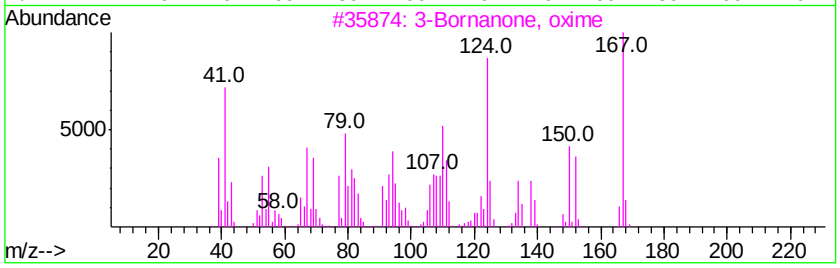
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.09 ng	112868	Phenanthrene-d10	11.23

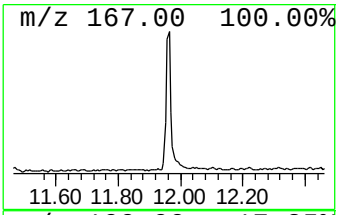
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
2	2-Bornanone oxime	167	C10H17NO	013559-66-5	53
3	3-Bornanone, oxime	167	C10H17NO	004514-87-8	50
4	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	47
5	Benzene, 1,1',1''-(1-ethanyl-2-y...	258	C20H18	001520-42-9	43

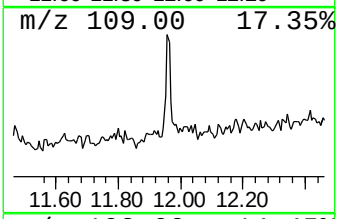


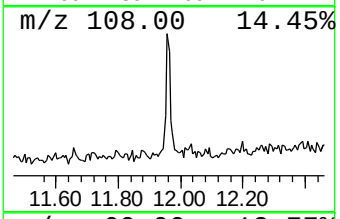


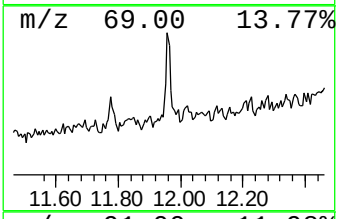


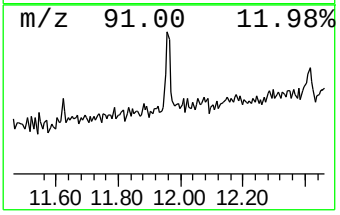












Tentatively Identified Compound (LSC) summary

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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...	4.91	2.8	ng	105062	1	6.72	760149	20.0
unknown6.49	6.49	81.3	ng	3090390	1	6.72	760149	20.0
Benzothiazole	8.28	12.0	ng	605956	2	8.00	1012030	20.0
2(3H)-Benzothiazo...	10.66	6.2	ng	333157	4	11.23	1082320	20.0
2-Mercaptobenzoth...	11.96	2.1	ng	112868	4	11.23	1082320	20.0