LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090117\
Data File : BF098236.D
Acq On : 1 Sep 2017 19:36
Operator : SJ/JU
Sample : I4963-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3831-PA3

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	4.904	476	479	489	rVB	76586	98513	2.84%	0.429%
2	5.328	546	551	554	rBV	1743485	1634033	47.07%	7.121%
3	6.357	722	726	739	rBV	1148454	1136218	32.73%	4.951%
4	6.492	744	749	752	rBV	2865357	2660902	76.64%	11.596%
5	6.716	784	787	791	rBV	940301	772070	22.24%	3.364%
6	6.875	810	814	817	rBV	2647036	2444000	70.40%	10.650%
7	7.286	879	884	887	rBV	2045772	2128919	61.32%	9.277%
8	8.004	1002	1006	1009	rBV	1065014	982059	28.29%	4.280%
9	8.281	1049	1053	1060	rBV	222941	208825	6.01%	0.910%
10	9.080	1184	1189	1192	rBV	3626309	3471799	100.00%	15.129%
11	9.751	1299	1303	1313	rBV	1086880	998164	28.75%	4.350%
12	10.545	1433	1438	1441	rBV	1712446	1649558	47.51%	7.188%
13	10.651	1453	1456	1464	rVB2	79459	89303	2.57%	0.389%
14	11.233	1551	1555	1559	rBV	952386	826770	23.81%	3.603%
15	11.957	1675	1678	1685	rVB	75721	92919	2.68%	0.405%
16	12.821	1820	1825	1828	rBV	2495149	2487288	71.64%	10.839%
17	13.868	1999	2003	2008	rBV	783690	710937	20.48%	3.098%
18	15.286	2240	2244	2253	rVB	447809	555320	16.00%	2.420%

Sum of corrected areas: 22947597

LSC Report - Integrated Chromatogram

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Operator : SJ/JU
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Misc :
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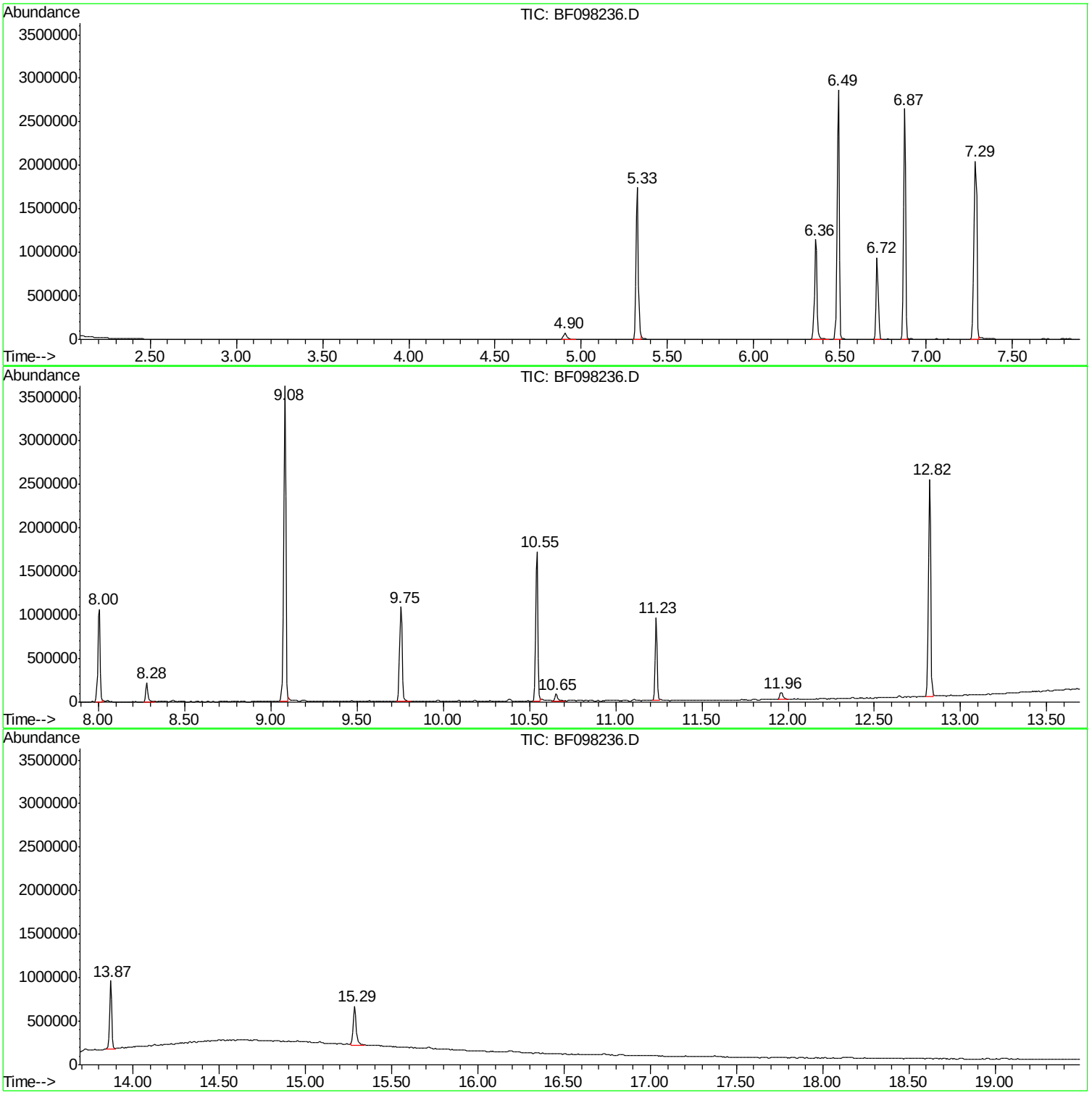
Instrument : BNA_F
ClientSampleId : 3831-PA3

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

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Data File : BF098236.D
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Operator : SJ/JU
Sample : I4963-12
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3831-PA3

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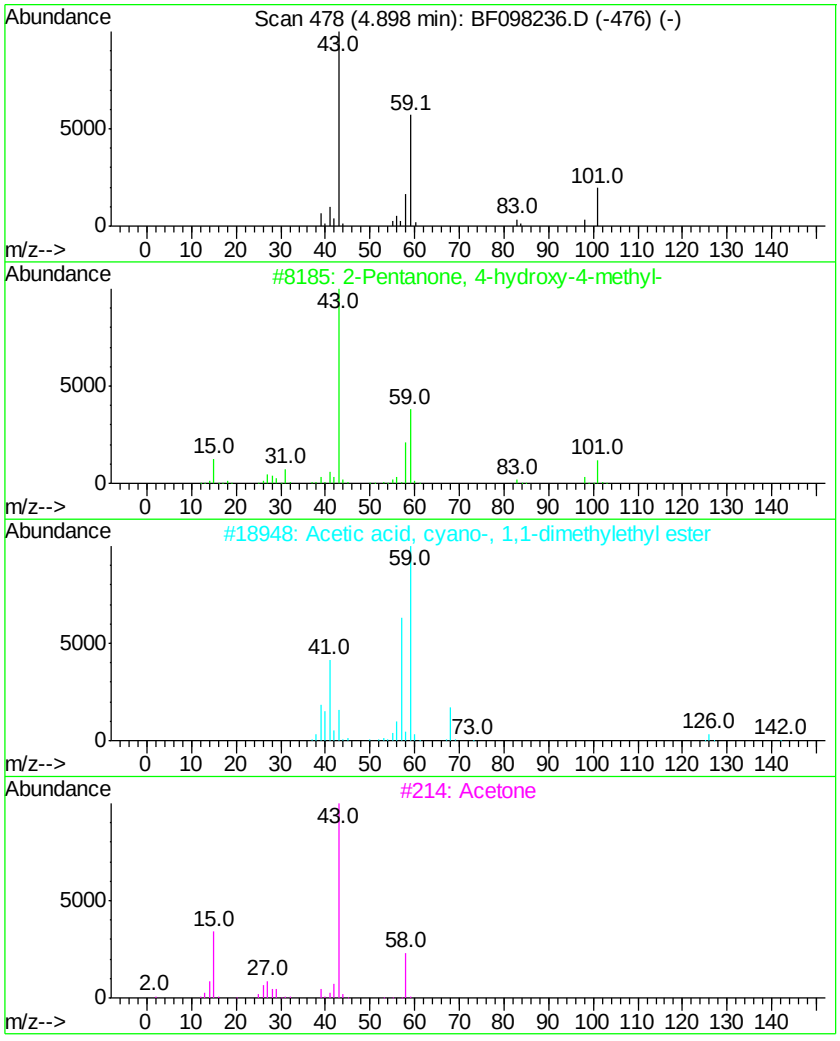
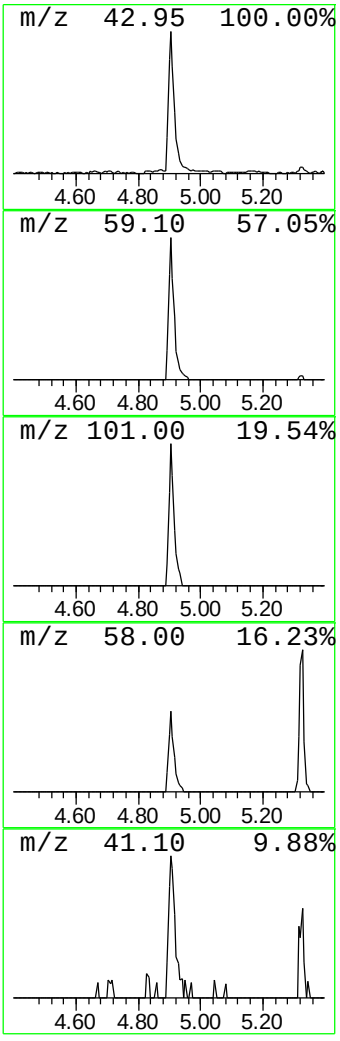
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.55 ng	98513	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	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Acetone	58	C3H6O	000067-64-1	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9





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Misc :
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Instrument : BNA_F
ClientSampleId : 3831-PA3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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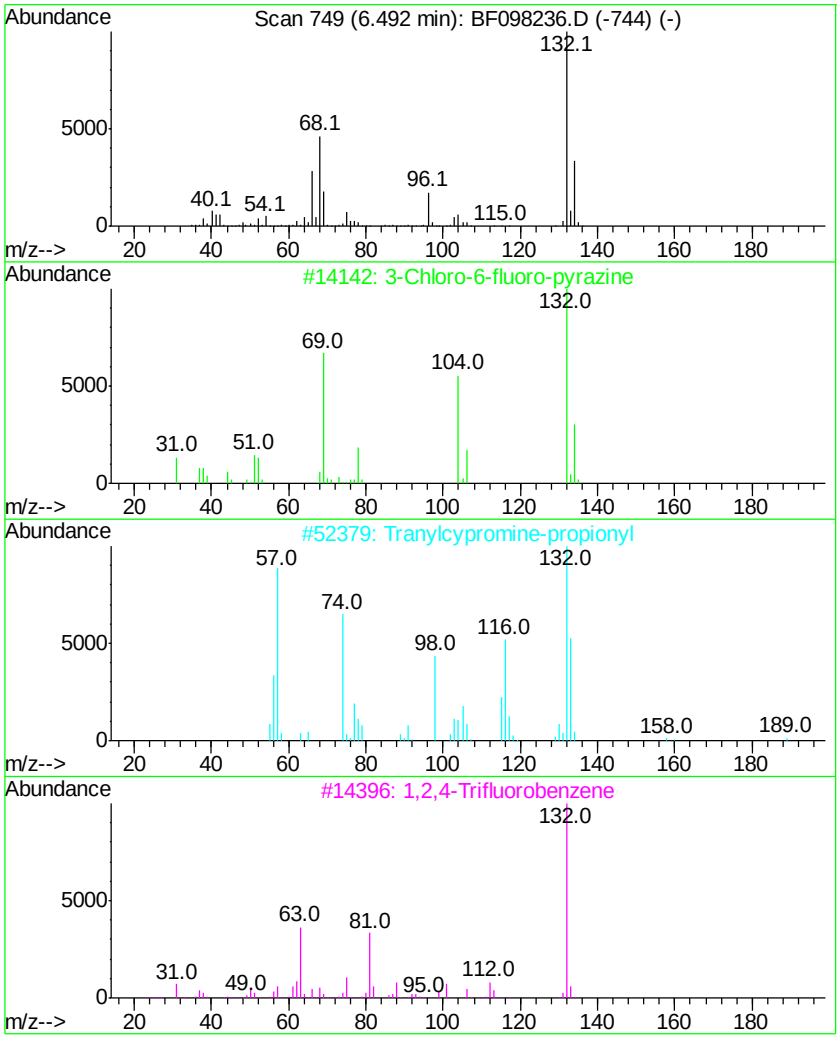
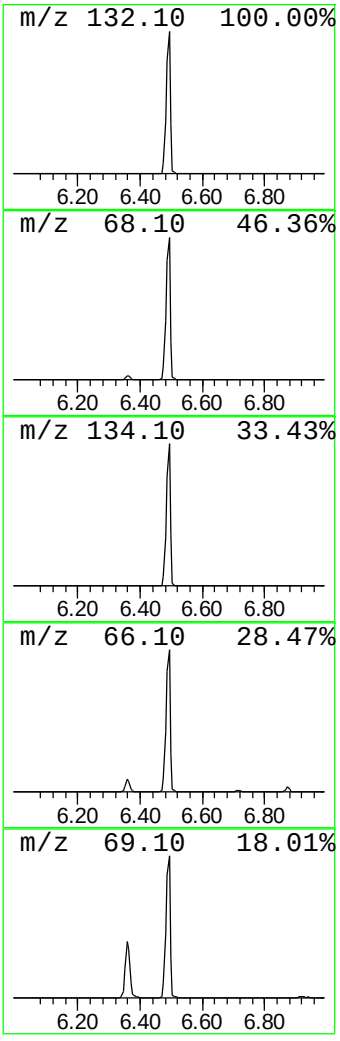
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	68.93 ng	2660900	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	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Instrument : BNA_F
ClientSampleId : 3831-PA3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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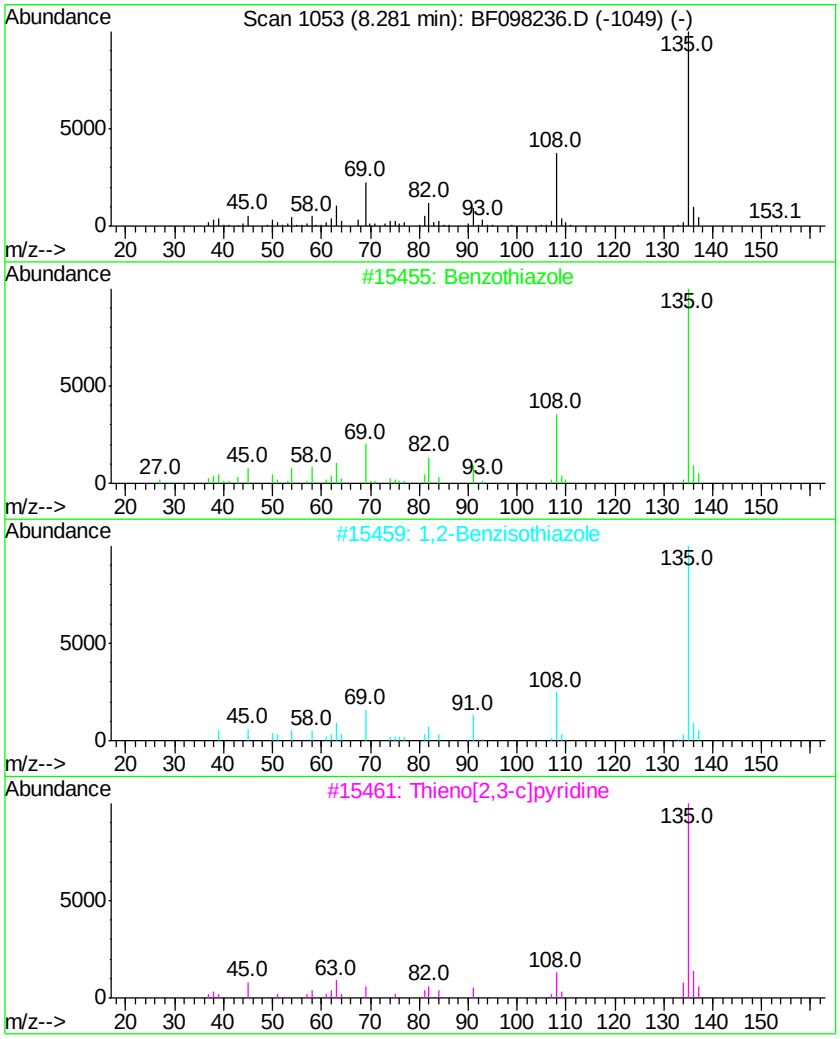
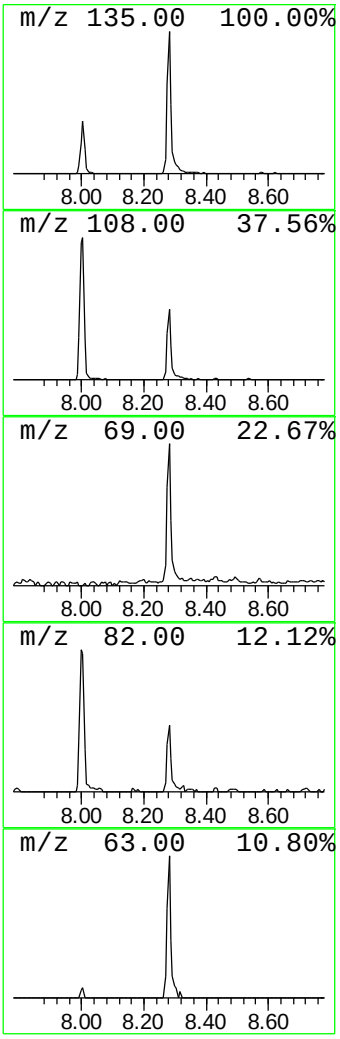
Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	4.25 ng	208825	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	87
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	83
4	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	78
5	Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	72





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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3831-PA3

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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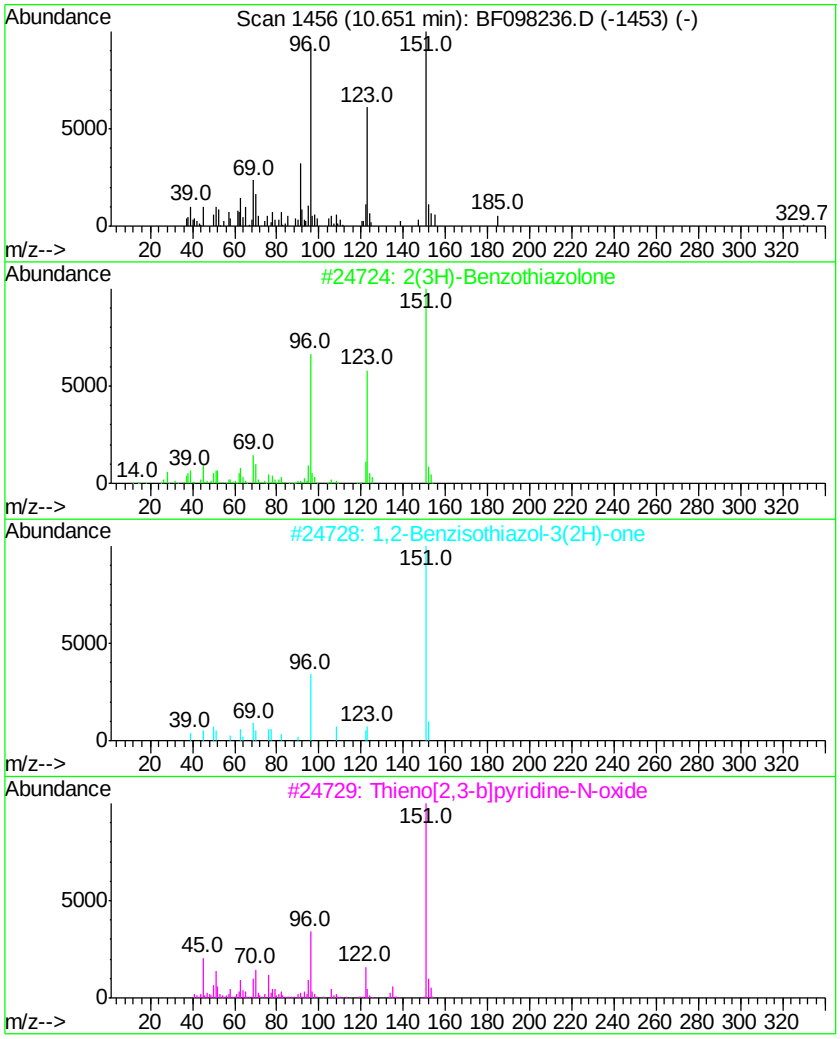
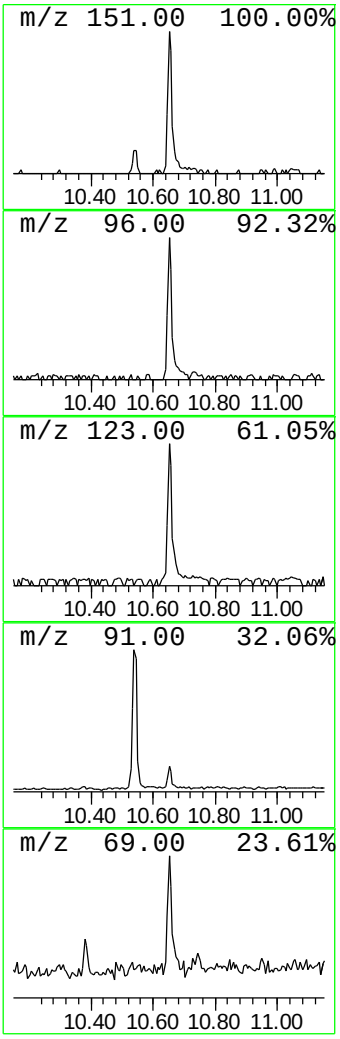
Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.16 ng	89303	Phenanthrene-d10	11.23

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	64
3	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	43
4	2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	41
5	1,2,4-Triazolo[4,3-a]pyridine-3(...	151	C6H5N3S	006952-68-7	38





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Misc :
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TIC Integration Parameters: LSCINT.P

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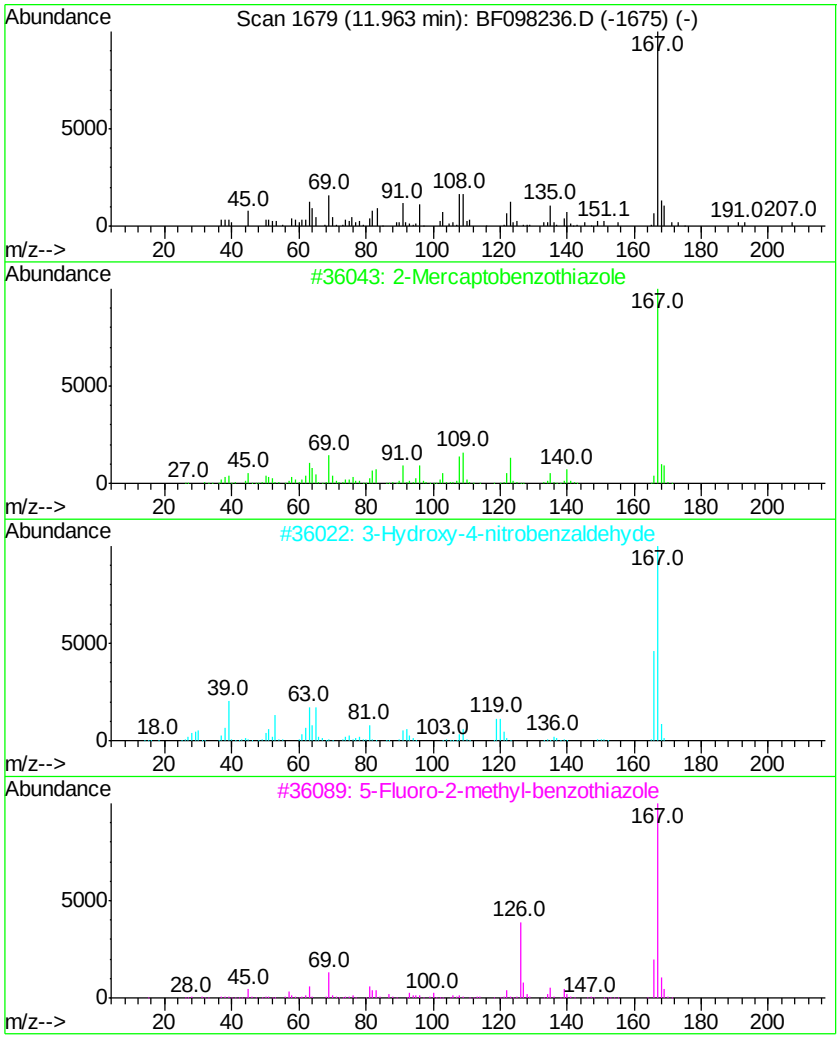
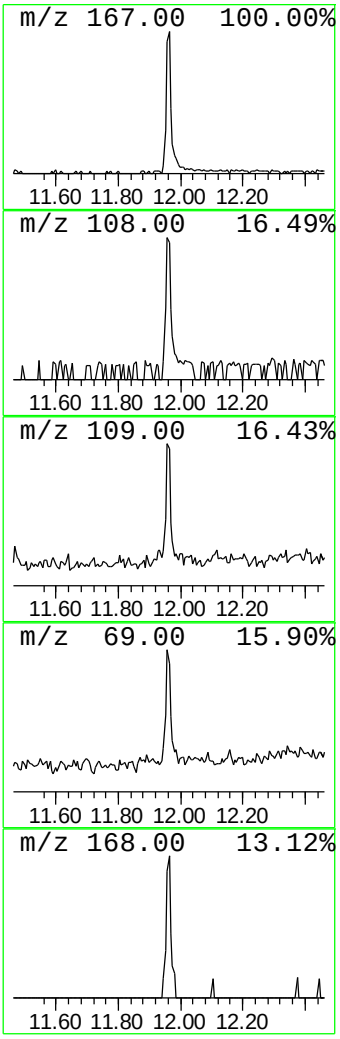
Peak Number 6 2-Mercaptobenzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.25 ng	92919	Phenanthrene-d10	11.23

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	50
3	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	50
4	1,3-Benzodioxole, 5-nitro-	167	C7H5NO4	002620-44-2	47
5	Alanine, N-acetyl-3-[(2-benzothi...	328	C12H12N2O3S3	159357-94-5	45





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
2-Pentanone, 4-hy...	4.90	2.5	ng	98513	1	6.72	772070	20.0
unknown6.49	6.49	68.9	ng	2660900	1	6.72	772070	20.0
Benzothiazole	8.28	4.3	ng	208825	2	8.00	982059	20.0
2(3H)-Benzothiazo...	10.65	2.2	ng	89303	4	11.23	826770	20.0
2-Mercaptobenzoth...	11.96	2.3	ng	92919	4	11.23	826770	20.0