LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099475.D
Acq On : 14 Oct 2017 14:27
Operator : SJ/JU
Sample : I5819-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3916-DB

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-BF092317.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	2.134	4	8	22	rVB	192289	249233	7.08%	1.112%
2	5.081	505	509	527	rVB	155629	197836	5.62%	0.882%
3	5.475	573	576	592	rBV	1437522	1498566	42.60%	6.684%
4	6.487	744	748	761	rBV	1040643	918560	26.11%	4.097%
5	6.628	767	772	775	rBV	2682152	2527902	71.86%	11.275%
6	6.851	807	810	814	rBV	769326	623602	17.73%	2.781%
7	7.010	833	837	840	rBV	2686866	2481634	70.54%	11.069%
8	7.422	902	907	910	rBV	1879283	1969892	56.00%	8.786%
9	8.134	1024	1028	1034	rBV	1051563	848123	24.11%	3.783%
10	8.416	1074	1076	1080	rVB	69303	57132	1.62%	0.255%
11	9.210	1206	1211	1214	rBV	3557871	3517866	100.00%	15.691%
12	9.886	1322	1326	1330	rBV2	1023685	904233	25.70%	4.033%
13	10.269	1388	1391	1394	rBV	59881	50547	1.44%	0.225%
14	10.680	1457	1461	1465	rBV	1670171	1728270	49.13%	7.709%
15	10.804	1478	1482	1485	rBV	428546	416307	11.83%	1.857%
16	11.186	1544	1547	1551	rVB	41127	37841	1.08%	0.169%
17	11.233	1552	1555	1557	rVB	61879	45560	1.30%	0.203%
18	11.374	1576	1579	1583	rVB	896029	796309	22.64%	3.552%
19	12.963	1844	1849	1852	rBV	2582697	2511911	71.40%	11.204%
20	13.980	2019	2022	2025	rBV	99472	85148	2.42%	0.380%
21	14.021	2025	2029	2038	rVV	483038	492702	14.01%	2.198%
22	15.492	2274	2279	2287	rVB	379977	460996	13.10%	2.056%

Sum of corrected areas: 22420170

LSC Report - Integrated Chromatogram

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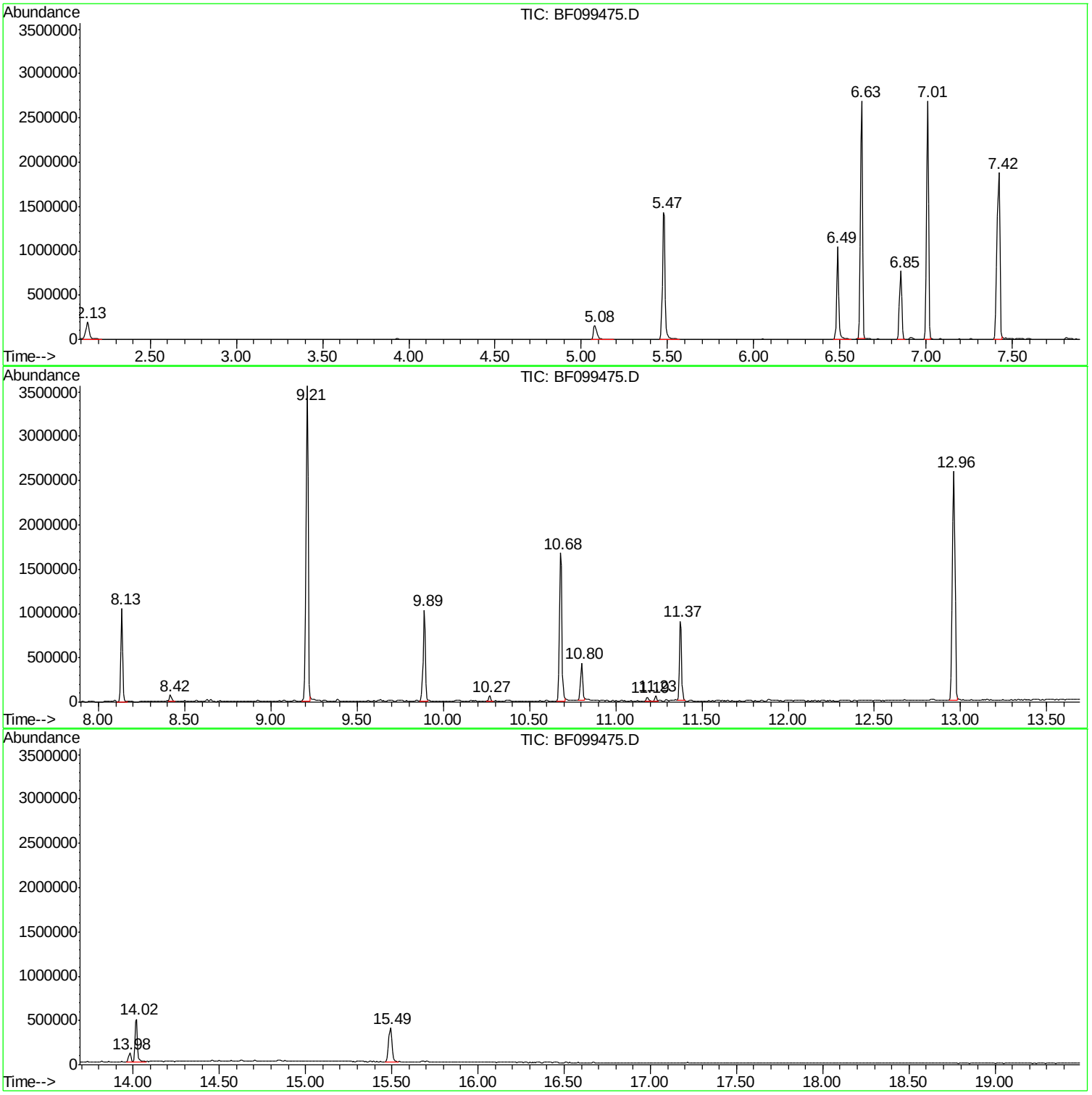
Instrument : BNA_F
ClientSampleId : 3916-DB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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Acq On : 14 Oct 2017 14:27
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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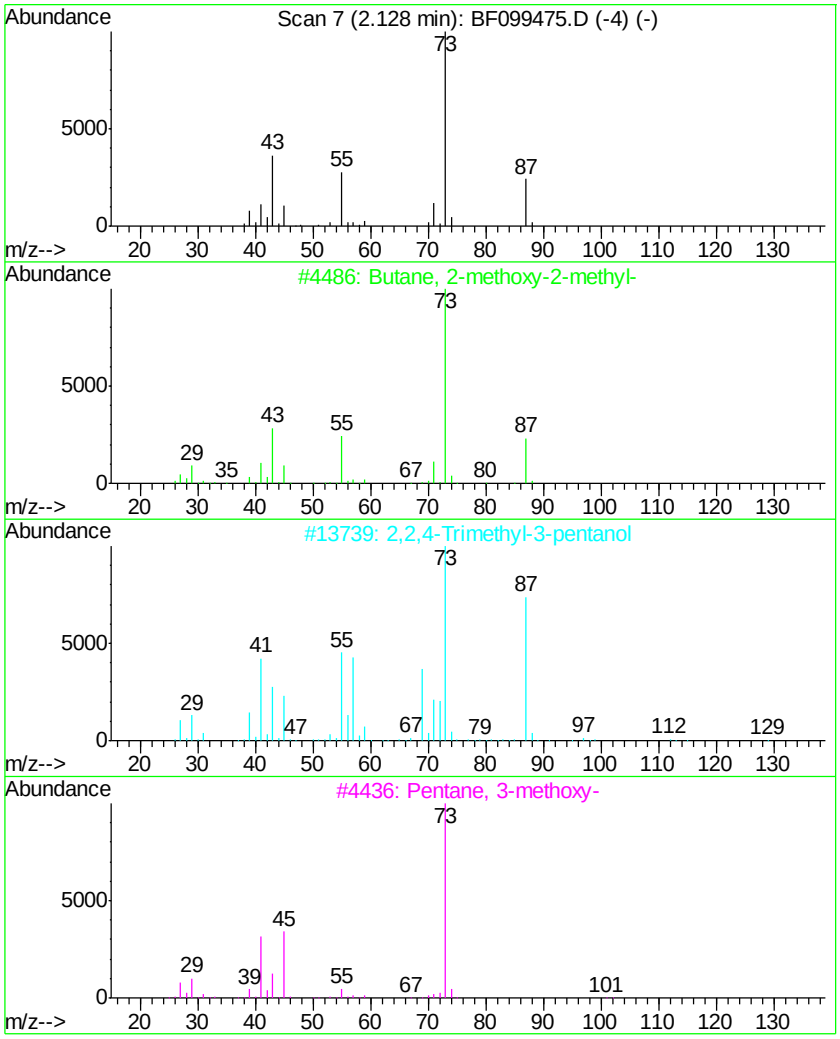
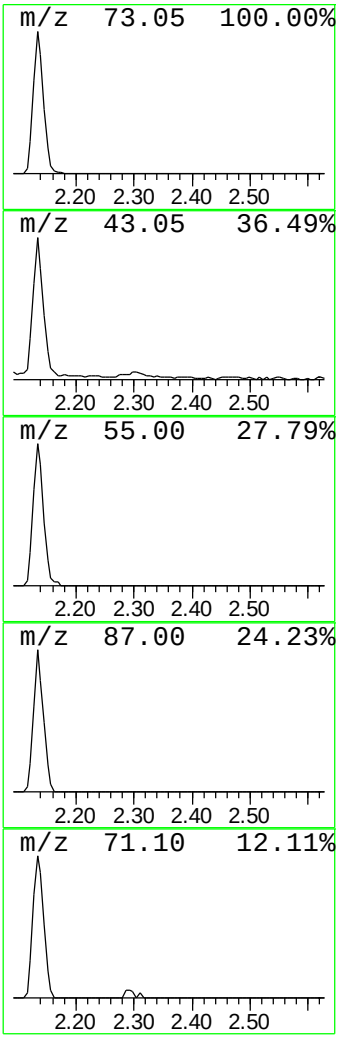
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	7.99 ng	249233	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Sample : I5819-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3916-DB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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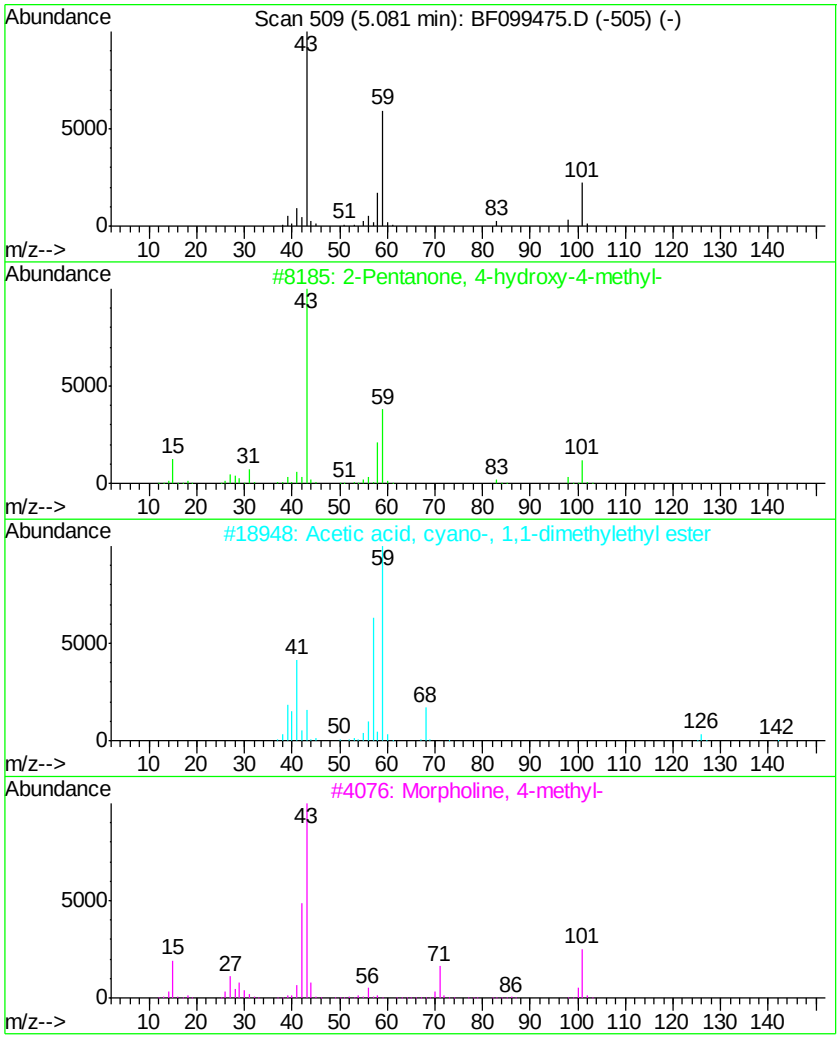
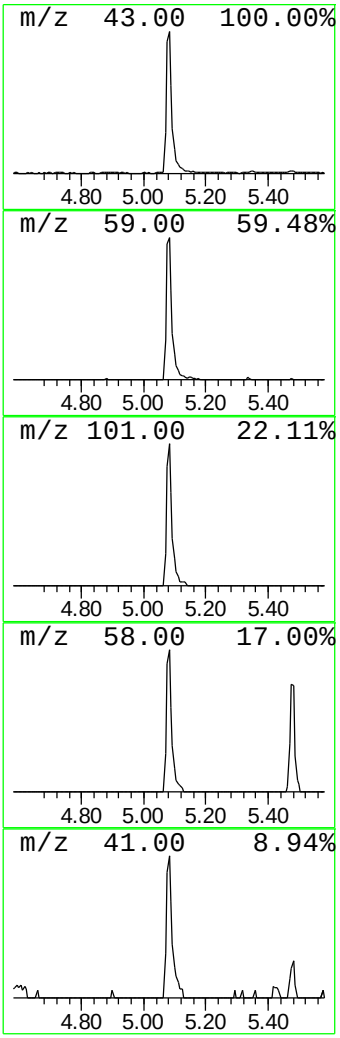
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	6.34 ng	197836	1,4-Dichlorobenzene-d4	6.85

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	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101417\
Data File : BF099475.D
Acq On : 14 Oct 2017 14:27
Operator : SJ/JU
Sample : I5819-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3916-DB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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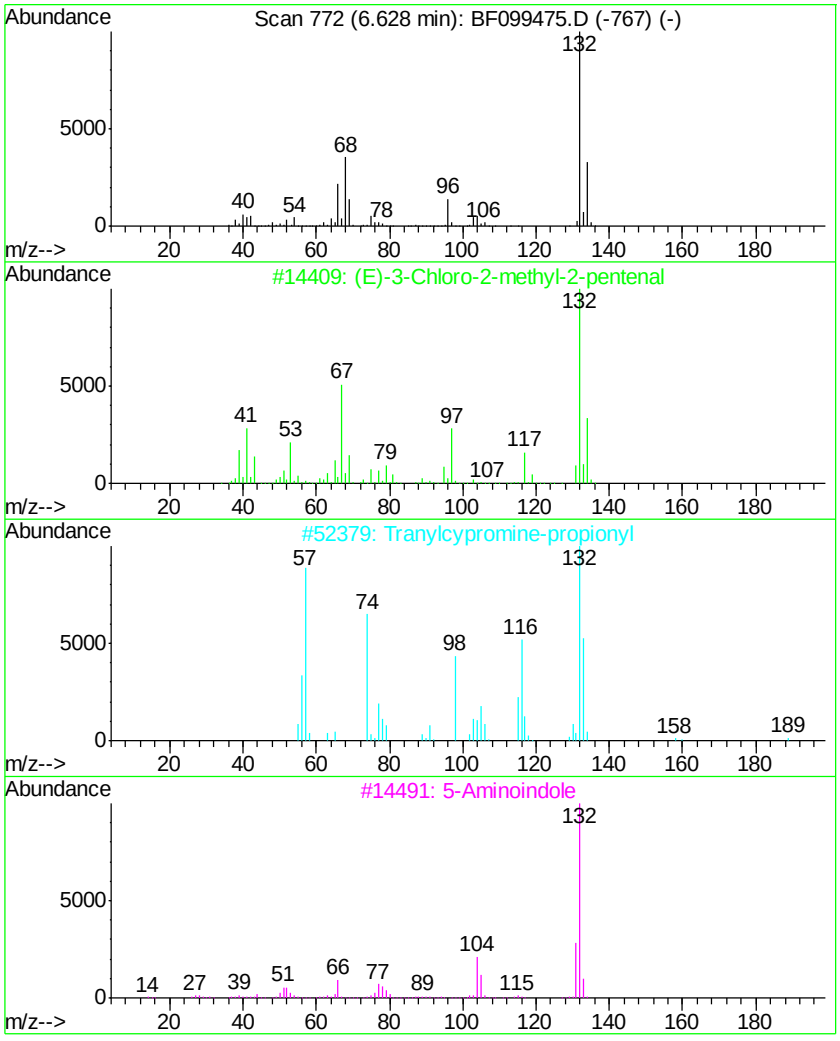
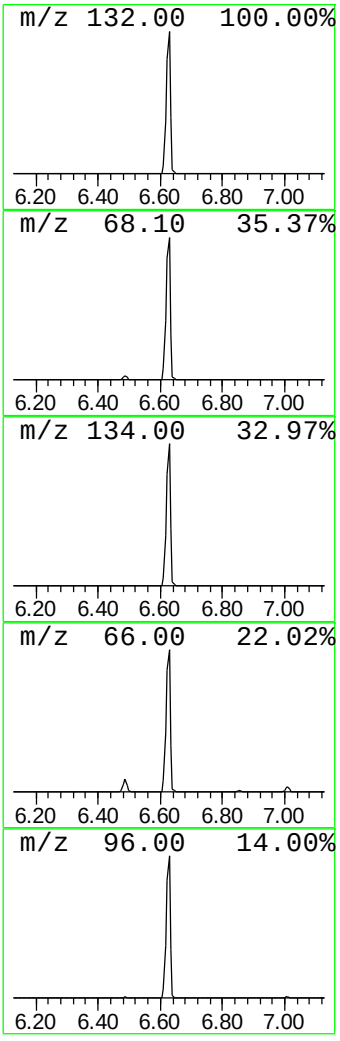
Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	81.07 ng	2527900	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3916-DB

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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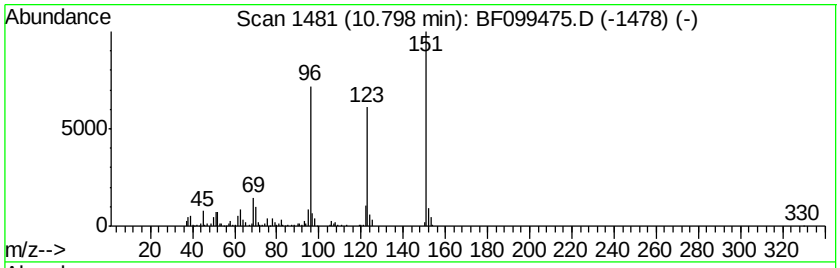
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

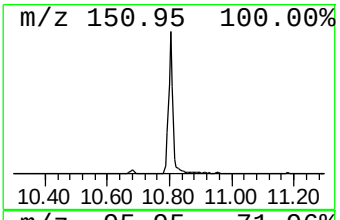
****

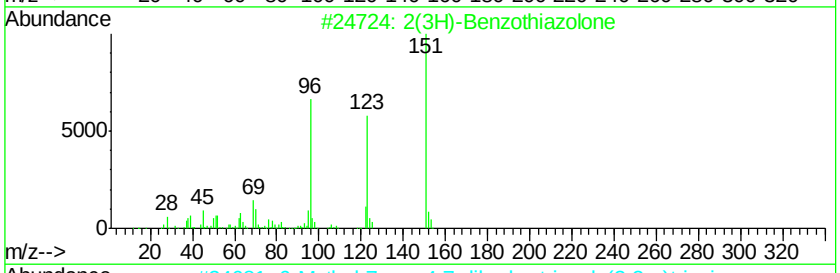
Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 3

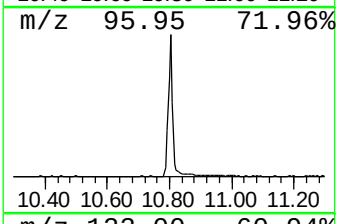
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	10.46 ng	416307	Phenanthrene-d10	11.37

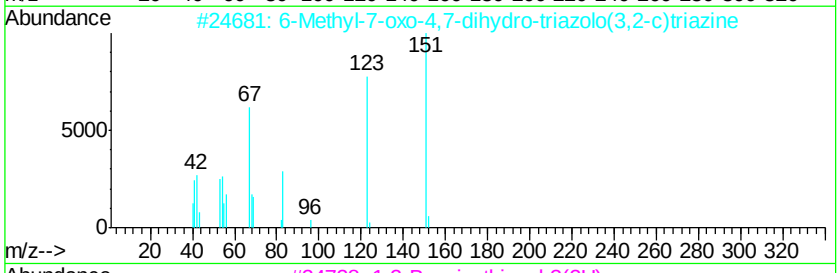
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
2	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	47
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	45
4	4-Mercaptoimidazo[4,5-c]pyridine	151	C6H5N3S	034550-51-1	38
5	2(3H)-Benzoxazolethione	151	C7H5NOS	002382-96-9	35

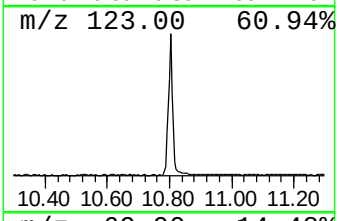


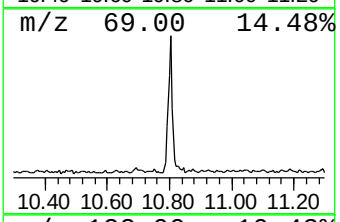


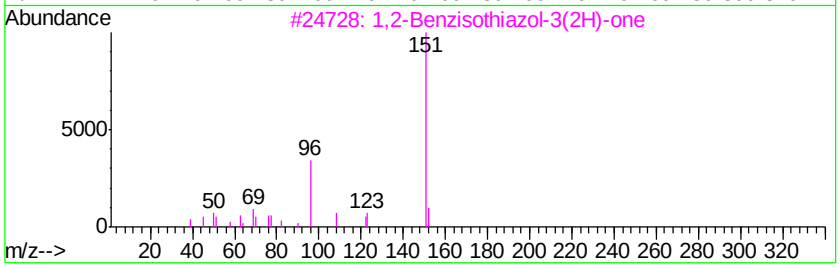


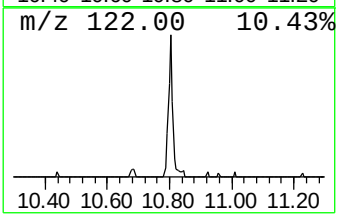












Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	8.0	ng	249233	1	6.85	623602	20.0
2-Pentanone, 4-hy...	5.08	6.3	ng	197836	1	6.85	623602	20.0
unknown6.63	6.63	81.1	ng	2527900	1	6.85	623602	20.0
2(3H)-Benzothiazo...	10.80	10.5	ng	416307	4	11.37	796309	20.0