LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041017\
Data File : BF094311.D
Acq On : 10 Apr 2017 15:16
Operator : SJ/MA
Sample : I2585-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1A

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-BF032217.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	3.969	350	354	360	rBV	271991	287391	5.31%	0.750%
2	4.393	422	426	435	rBV	2195393	2108449	38.93%	5.502%
3	5.469	603	609	618	rBV	1279668	1421677	26.25%	3.710%
4	5.593	623	630	634	rBV	3324594	3798226	70.14%	9.911%
5	5.834	667	671	675	rBV	974925	1013789	18.72%	2.645%
6	5.934	682	688	691	rBV	2107361	2224928	41.08%	5.805%
7	6.016	697	702	706	rVB	3243905	3671434	67.79%	9.580%
8	6.293	744	749	750	rBV2	101104	62304	1.15%	0.163%
9	6.493	775	783	786	rBV	2508914	3093079	57.11%	8.071%
10	6.687	804	816	819	rBV	140913	285712	5.28%	0.746%
11	7.075	878	882	889	rVV2	66960	110226	2.04%	0.288%
12	7.251	904	912	920	rBV3	129793	220847	4.08%	0.576%
13	7.340	920	927	931	rBV	1373719	1355571	25.03%	3.537%
14	7.669	980	983	988	rVB	254895	260542	4.81%	0.680%
15	7.840	1003	1012	1015	rBV2	35639	84847	1.57%	0.221%
16	8.134	1057	1062	1066	rBV2	58218	67830	1.25%	0.177%
17	8.669	1143	1153	1156	rVB	4406592	5415552	100.00%	14.131%
18	8.839	1178	1182	1187	rBV2	90058	115905	2.14%	0.302%
19	9.157	1232	1236	1244	rBV	122650	146069	2.70%	0.381%
20	9.481	1284	1291	1295	rBV2	1363142	1473684	27.21%	3.845%
21	10.028	1378	1384	1387	rBV2	56163	62004	1.14%	0.162%
22	10.463	1450	1458	1461	rBV	2386865	2843485	52.51%	7.419%
23	10.604	1477	1482	1485	rBV2	59051	61927	1.14%	0.162%
24	10.657	1485	1491	1493	rBV3	49109	64731	1.20%	0.169%
25	11.304	1594	1601	1604	rBV	1363971	1386142	25.60%	3.617%
26	12.033	1721	1725	1733	rBV2	63341	94927	1.75%	0.248%
27	13.098	1900	1906	1911	rVB2	45734	55332	1.02%	0.144%
28	13.286	1928	1938	1941	rBV2	3579607	4550210	84.02%	11.873%
29	14.551	2148	2153	2157	rBV	1122895	1189375	21.96%	3.103%
30	16.180	2425	2430	2435	rBV	709414	798305	14.74%	2.083%

Sum of corrected areas: 38324500

LSC Report - Integrated Chromatogram

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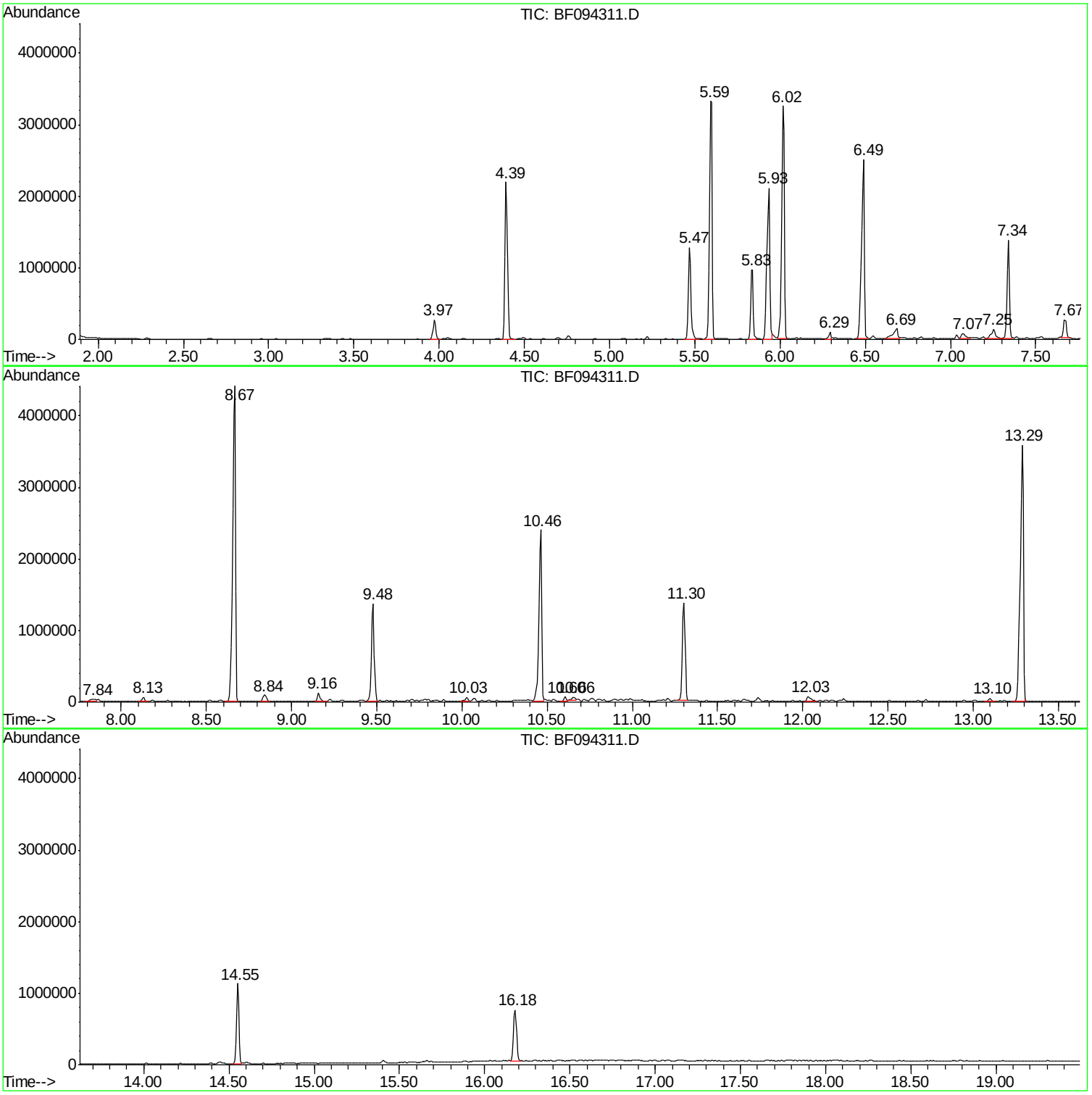
Operator : SJ/MA
Sample : I2585-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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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Data File : BF094311.D
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

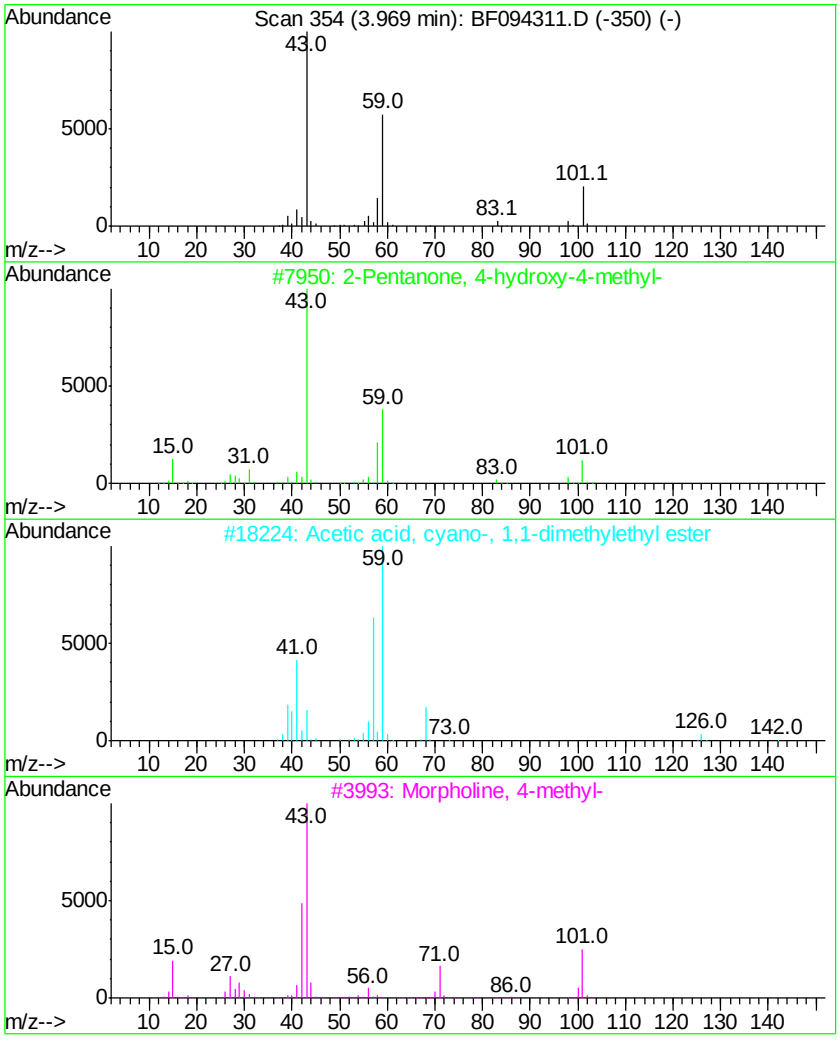
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

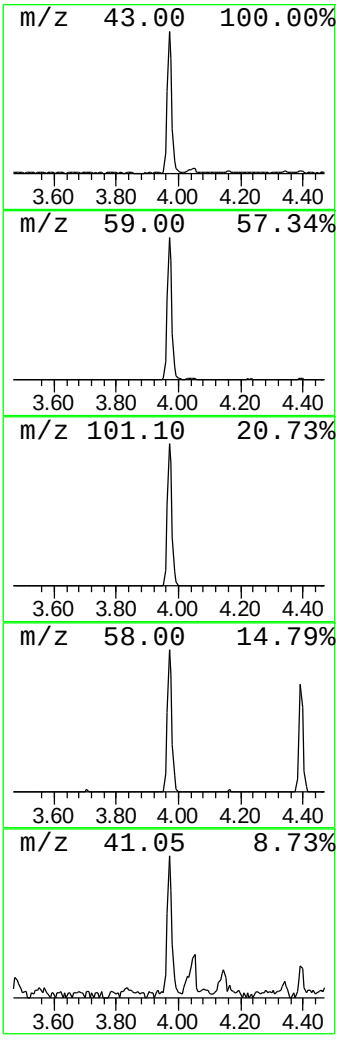
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.97	5.67 ng	287391	1,4-Dichlorobenzene-d4	5.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041017\
Data File : BF094311.D
Acq On : 10 Apr 2017 15:16
Operator : SJ/MA
Sample : I2585-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

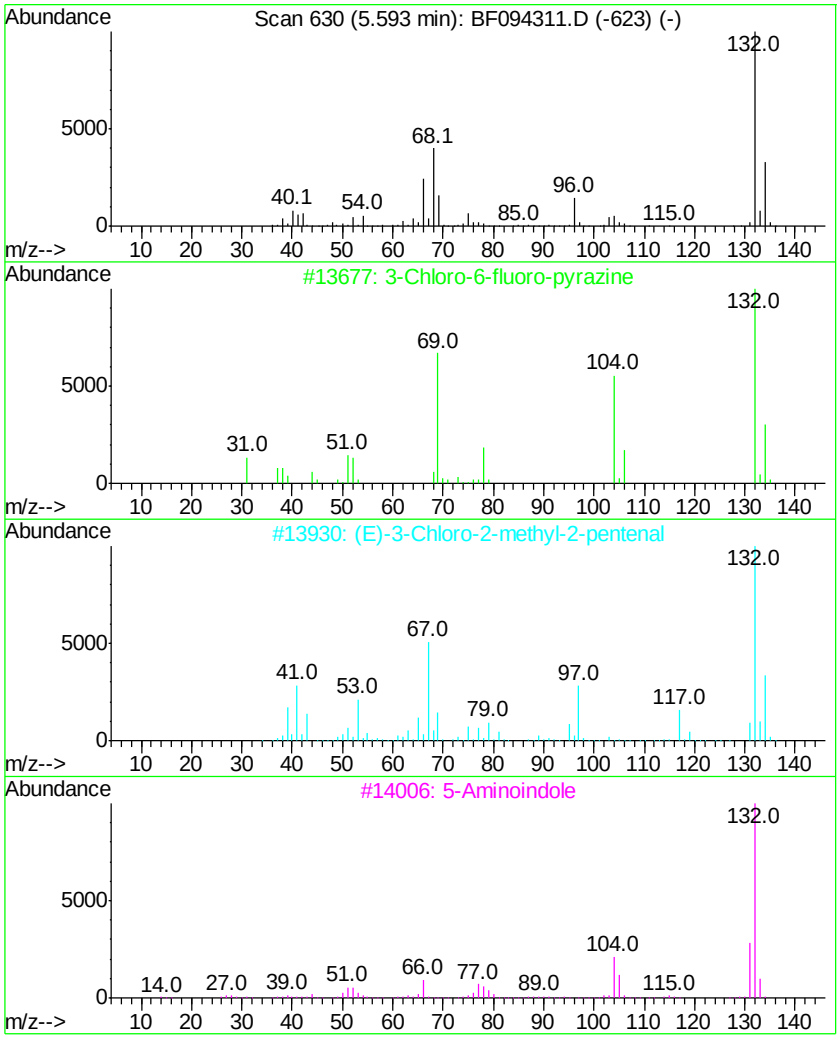
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

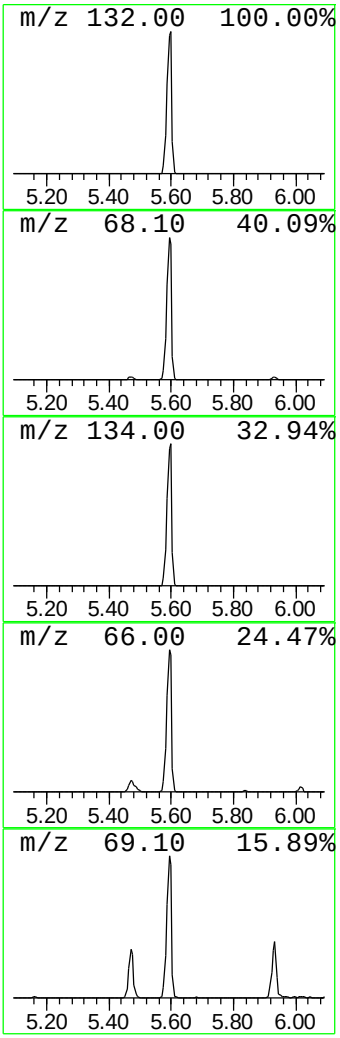
****

Peak Number 2 unknown5.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	74.93 ng	3798230	1,4-Dichlorobenzene-d4	5.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Sample : I2585-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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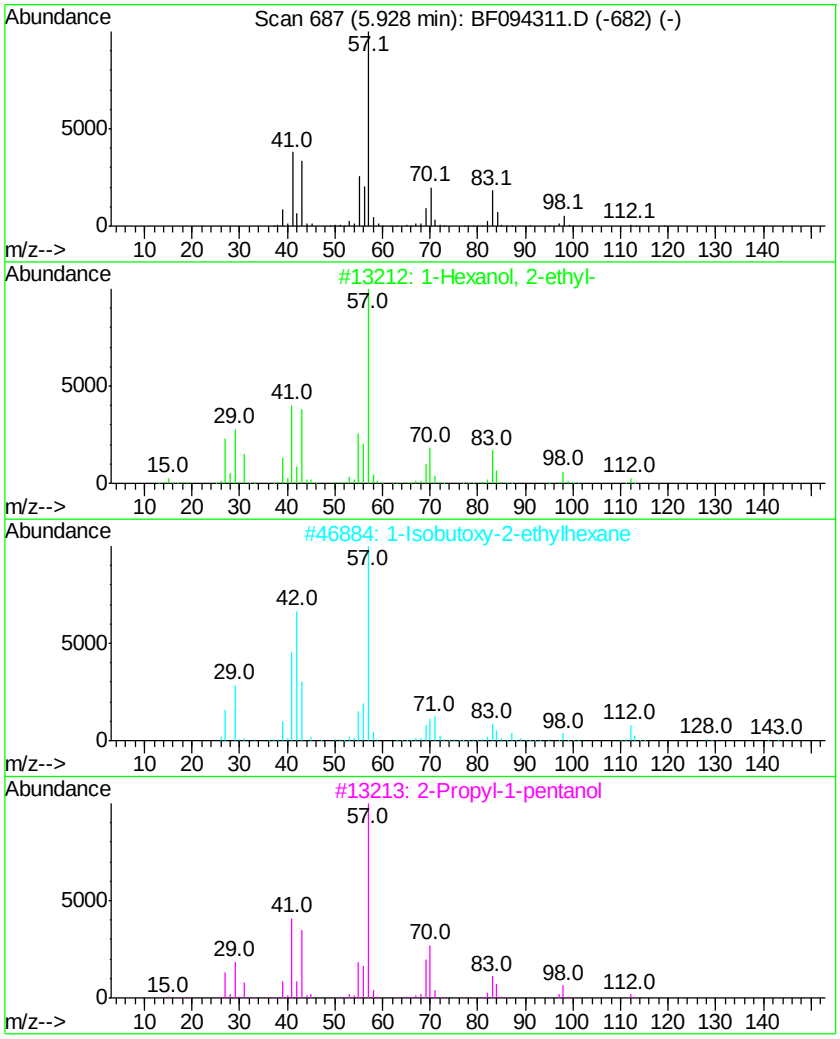
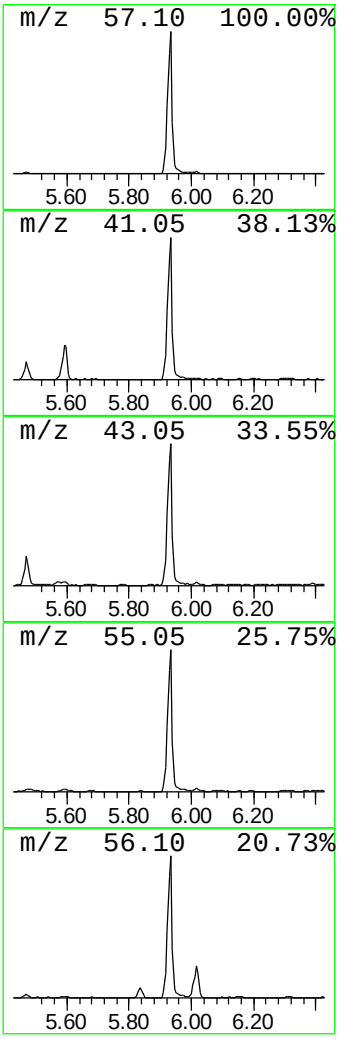
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	43.89 ng	2224930	1,4-Dichlorobenzene-d4	5.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	dl-2-Ethylhexyl chloroformate	192	C9H17ClO2	024468-13-1	50
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50





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Sample : I2585-03
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Instrument : BNA_F
ClientSampleId : 1A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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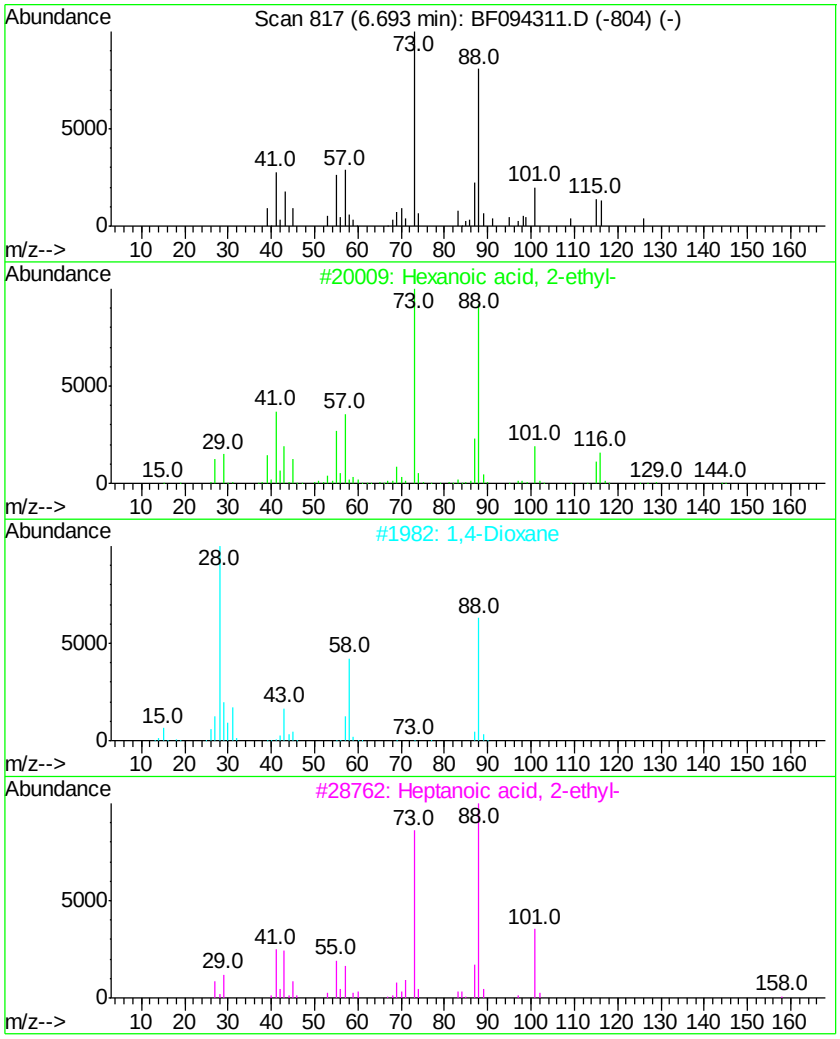
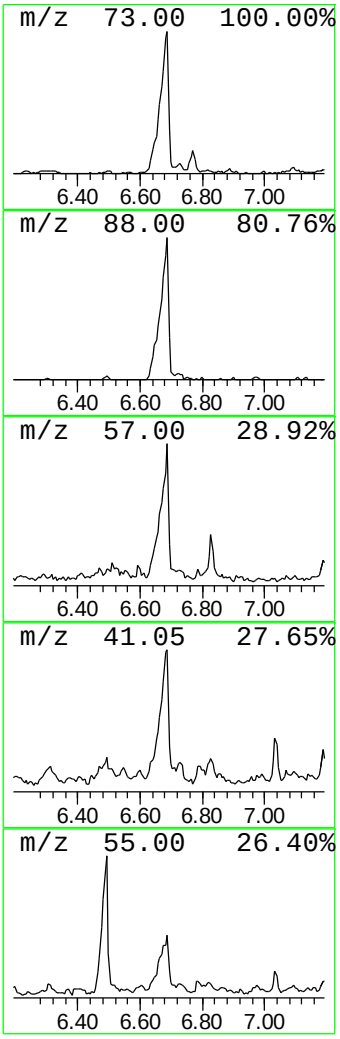
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	4.22 ng	285712	Naphthalene-d8	7.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	1,4-Dioxane	88	C4H8O2	000123-91-1	43
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
4	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	33
5	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	28





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Operator : SJ/MA
Sample : I2585-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

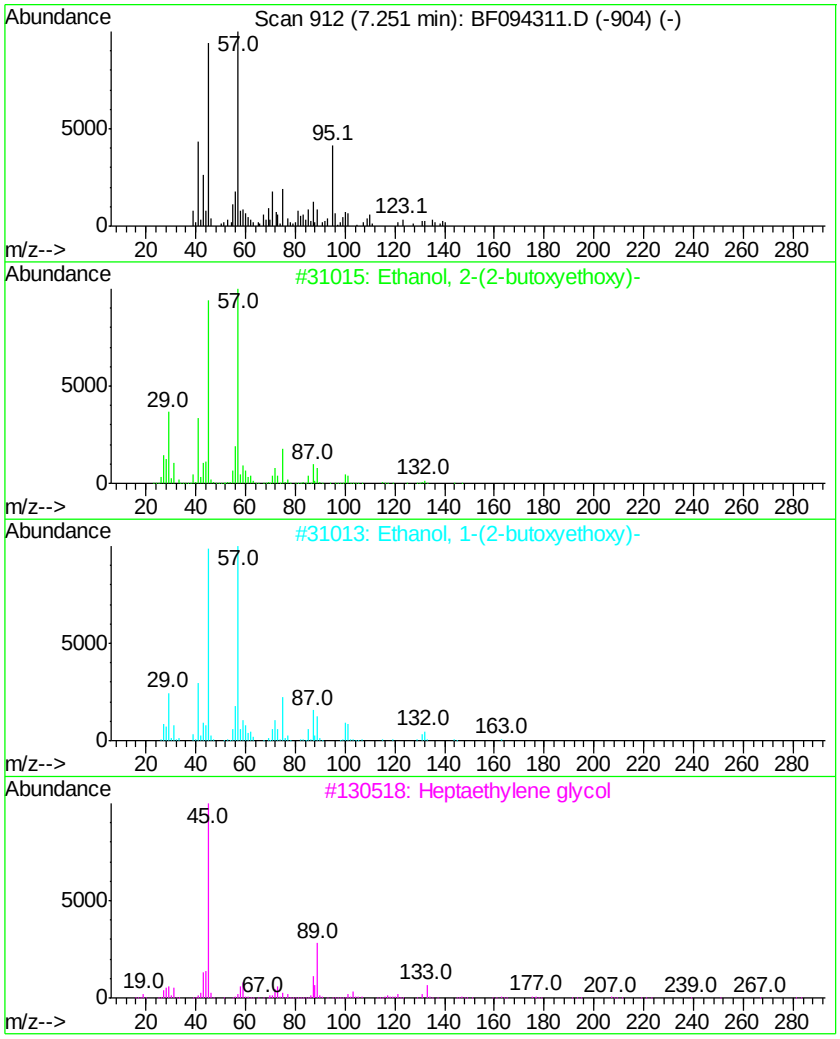
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

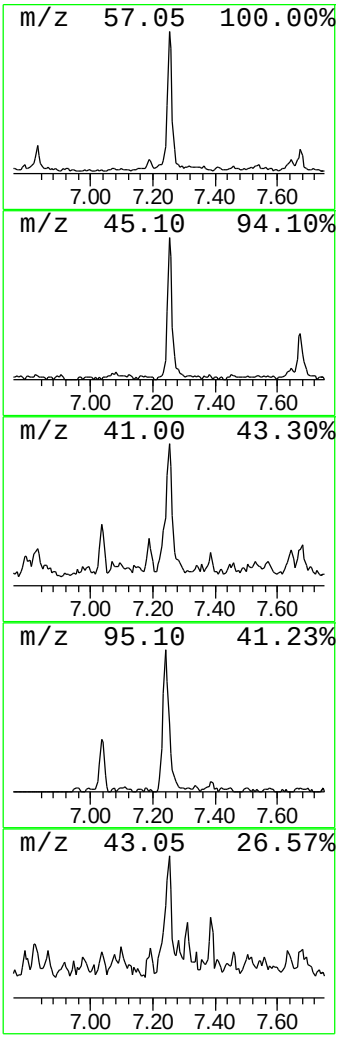
****

Peak Number 6 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.25	3.26 ng	220847	Naphthalene-d8	7.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	52
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
3	Heptaethylene glycol	326	C14H30O8	005617-32-3	43
4	Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	40
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	38





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Instrument : BNA_F
ClientSampleId : 1A

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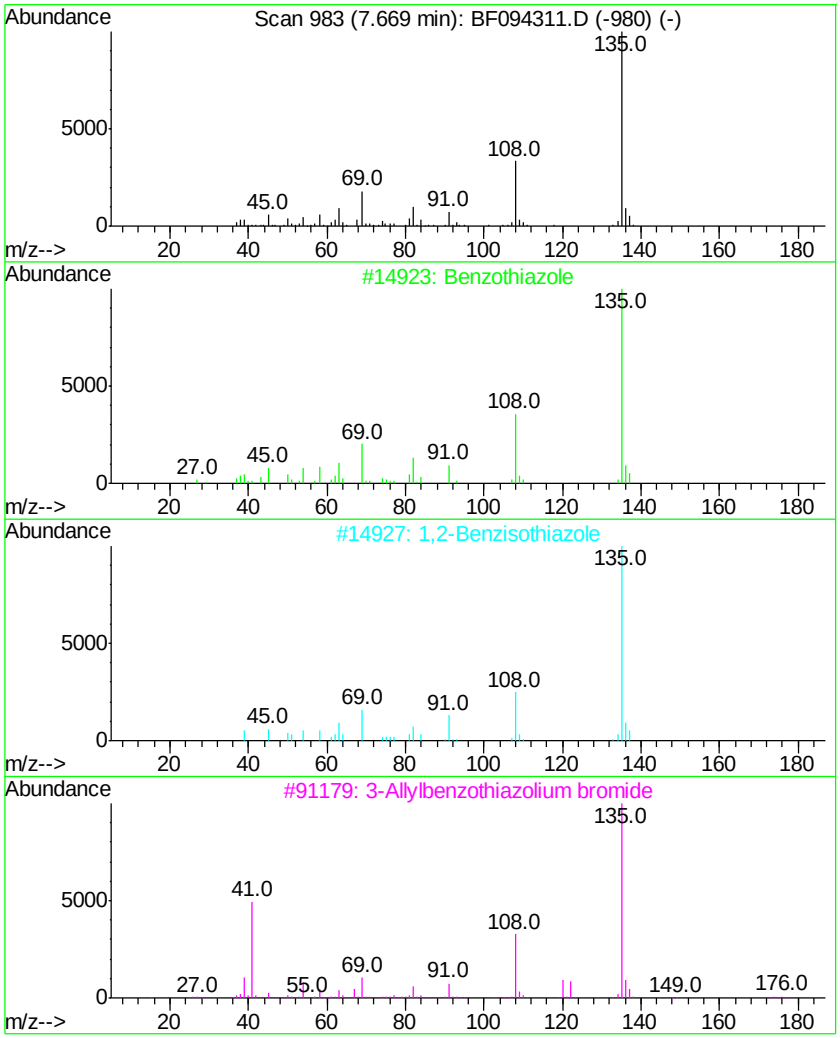
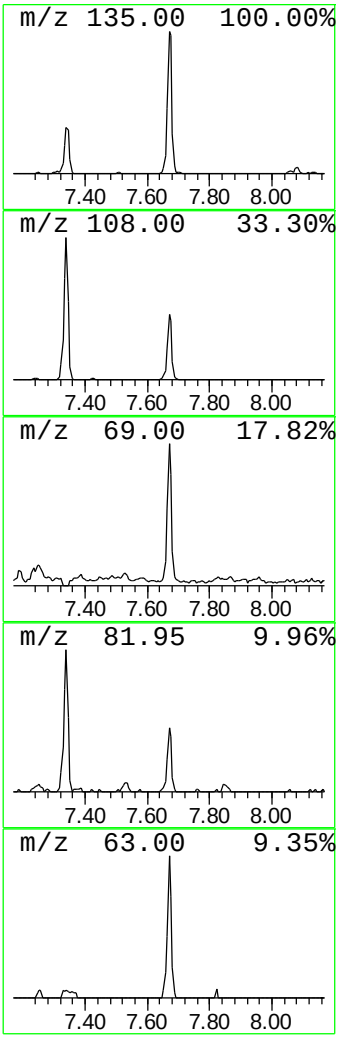
Peak Number 7 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	3.84 ng	260542	Naphthalene-d8	7.34

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	91
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	83
4	2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	72
5	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	58





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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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...	3.97	5.7	ng	287391	1	5.84	1013790	20.0
unknown5.59	5.59	74.9	ng	3798230	1	5.84	1013790	20.0
1-Hexanol, 2-ethyl-	5.93	43.9	ng	2224930	1	5.84	1013790	20.0
Hexanoic acid, 2-...	6.69	4.2	ng	285712	2	7.34	1355570	20.0
Ethanol, 2-(2-but...	7.25	3.3	ng	220847	2	7.34	1355570	20.0
Benzothiazole	7.67	3.8	ng	260542	2	7.34	1355570	20.0