LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030817\
Data File : BF093433.D
Acq On : 8 Mar 2017 17:29
Operator : SJ/MA
Sample : I2099-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 39B-9-11

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-BF030717.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	1.955	4	6	13	rVB	85976	121346	2.08%	0.240%
2	4.916	263	265	278	rBV	657457	1328404	22.75%	2.623%
3	5.361	301	304	320	rBV	4715234	5811383	99.53%	11.473%
4	6.413	393	396	399	rBV	4093805	5732825	98.18%	11.318%
5	6.539	404	407	409	rBV	4018161	5397206	92.43%	10.655%
6	6.756	424	426	429	rBV	846801	1109039	18.99%	2.190%
7	6.916	438	440	443	rBV	4008888	3926852	67.25%	7.753%
8	7.339	474	477	479	rBV	3588718	3659554	62.68%	7.225%
9	8.047	537	539	542	rBV	1012889	1425780	24.42%	2.815%
10	9.133	631	634	636	rBV	5088003	5838922	100.00%	11.528%
11	9.533	666	669	671	rBV	333102	417233	7.15%	0.824%
12	9.739	679	687	691	rBV	224798	569306	9.75%	1.124%
13	9.808	691	693	695	rVB	1347447	1594439	27.31%	3.148%
14	10.230	726	730	734	rBV	124729	153989	2.64%	0.304%
15	10.596	759	762	765	rBV	2887587	3124553	53.51%	6.169%
16	10.699	769	771	776	rVB	122480	168020	2.88%	0.332%
17	11.145	808	810	815	rVB	70295	115901	1.98%	0.229%
18	11.282	820	822	825	rBV	1261606	1643795	28.15%	3.245%
19	12.871	958	961	964	rBV	4136734	5038657	86.29%	9.948%
20	13.762	1037	1039	1048	rBV	210422	303309	5.19%	0.599%
21	13.934	1051	1054	1056	rVV	1211686	1585848	27.16%	3.131%
22	15.339	1174	1177	1187	rBV	1089442	1518273	26.00%	2.997%
23	17.351	1349	1353	1358	rVB3	23274	67369	1.15%	0.133%

Sum of corrected areas: 50652003

LSC Report - Integrated Chromatogram

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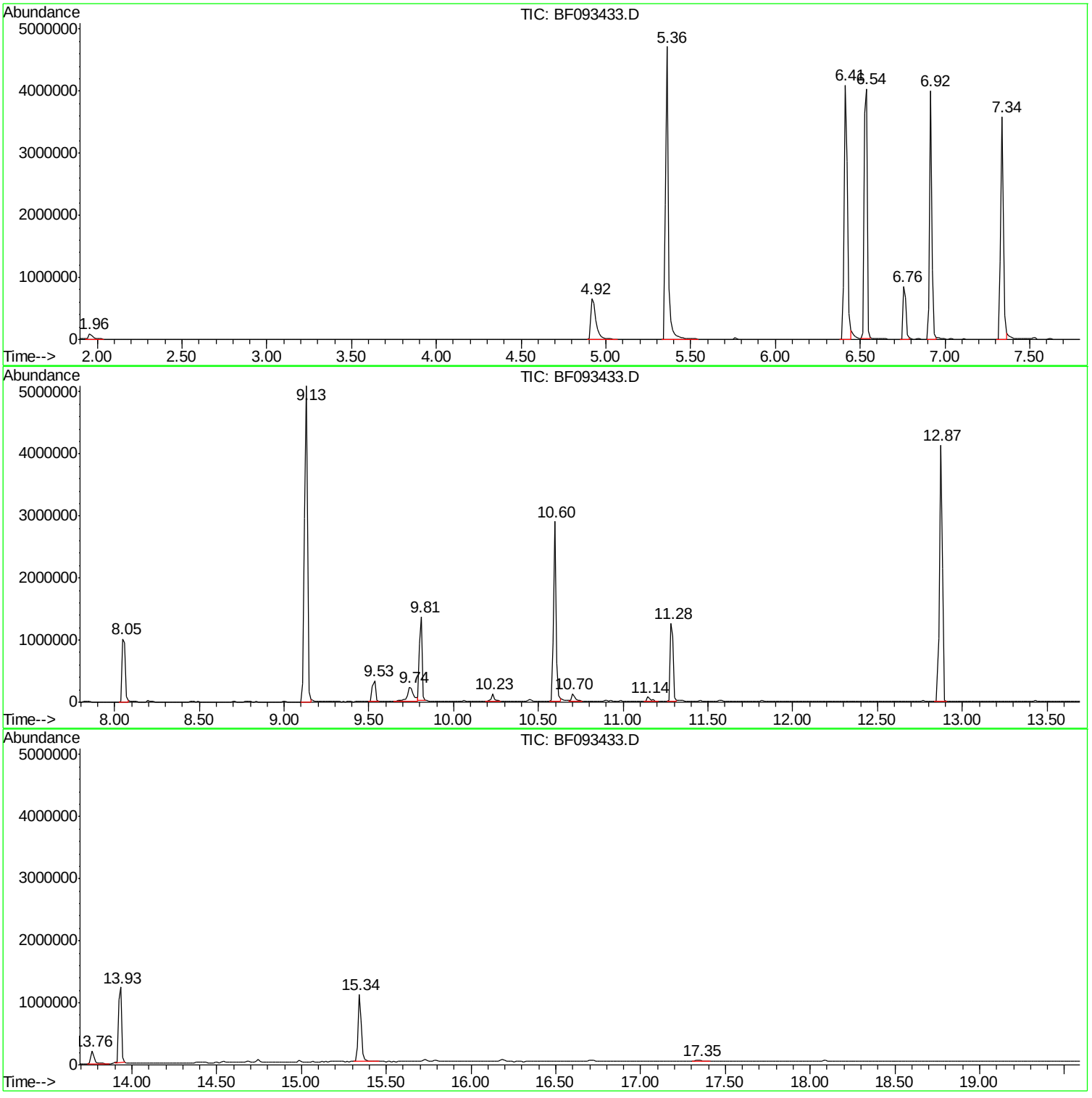
Instrument : BNA_F
ClientSampleId : 39B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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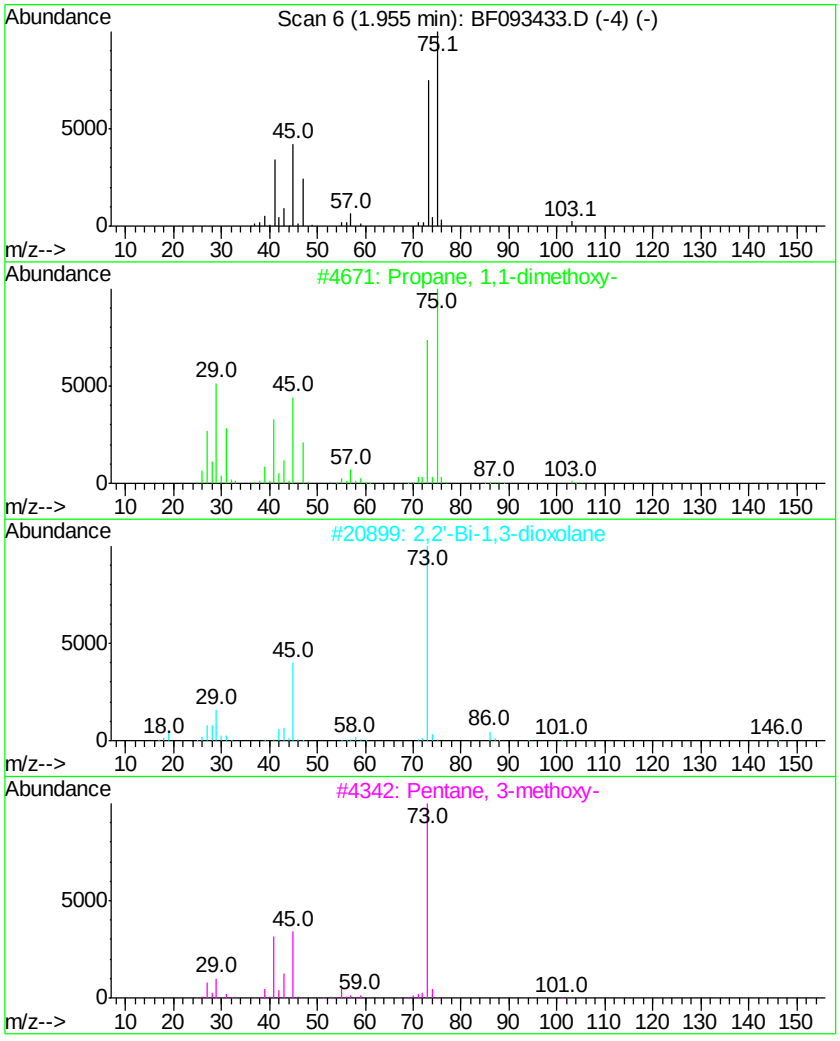
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

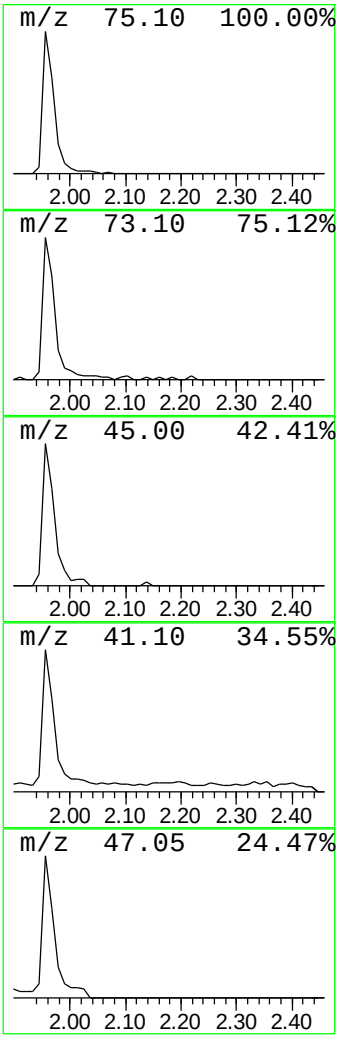
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.96	2.19 ng	121346	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	16
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
4	2-(3-Bromopropyl)-[1,3]dioxolane	194	C6H11BrO2	062563-07-9	10
5	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9





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Instrument : BNA_F
ClientSampleId : 39B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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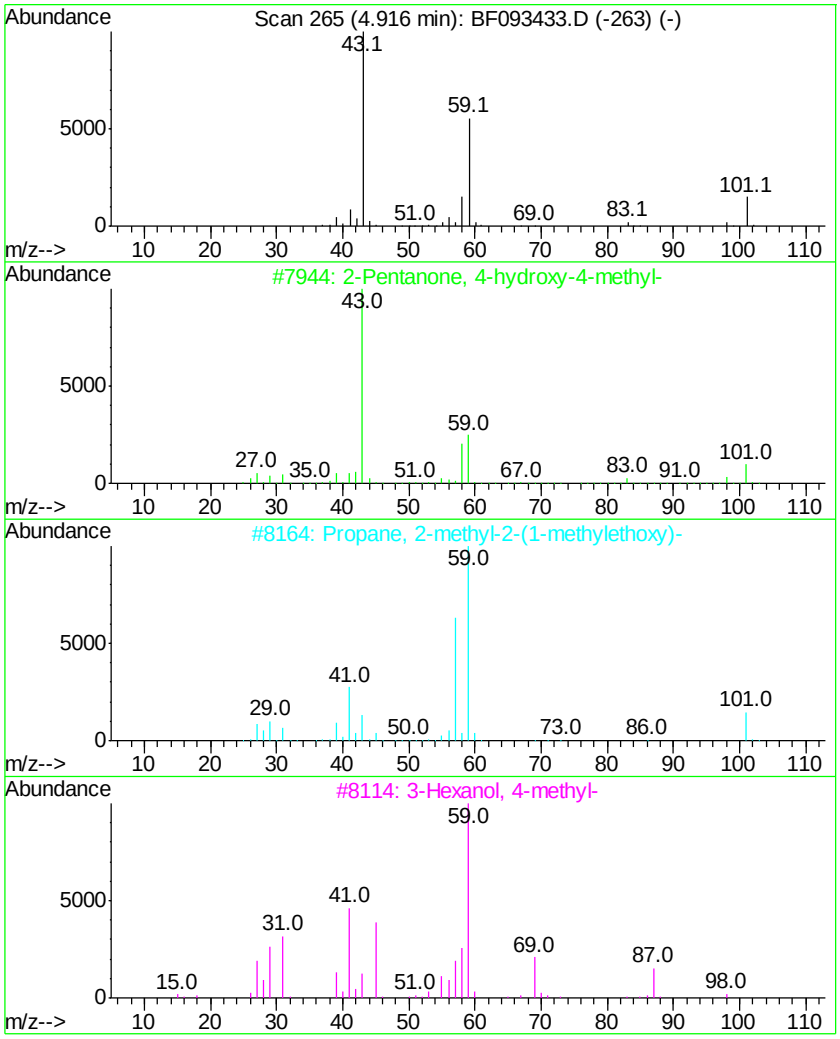
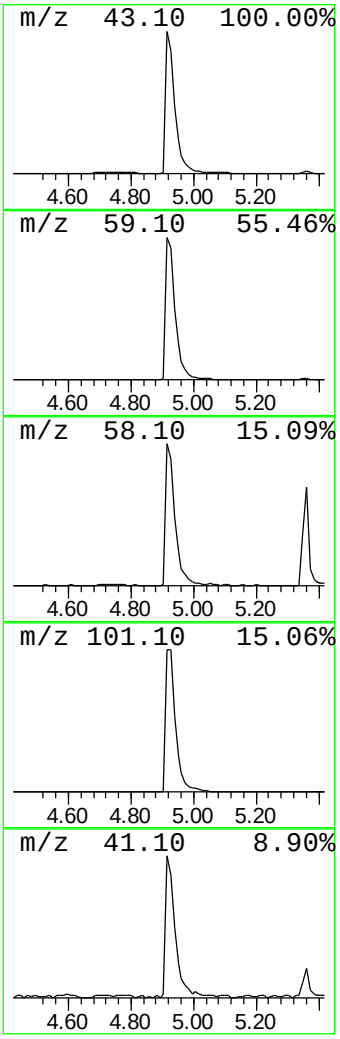
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	23.96 ng	1328400	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Operator : SJ/MA
Sample : I2099-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 39B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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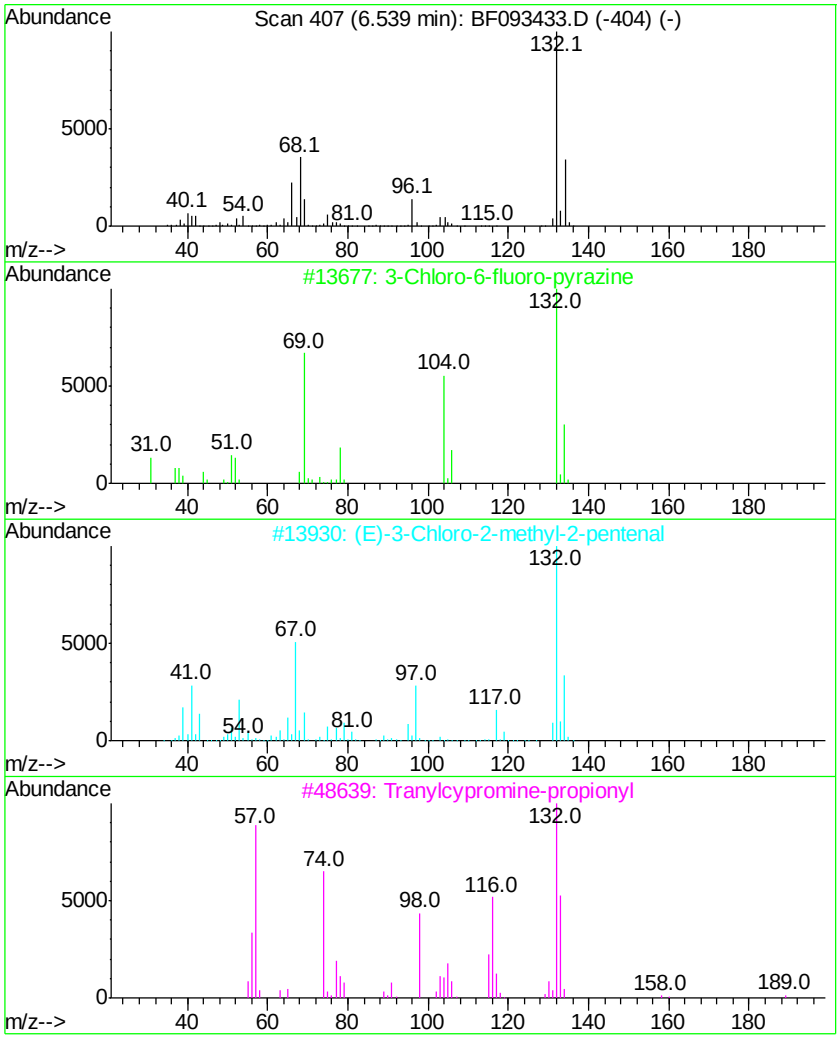
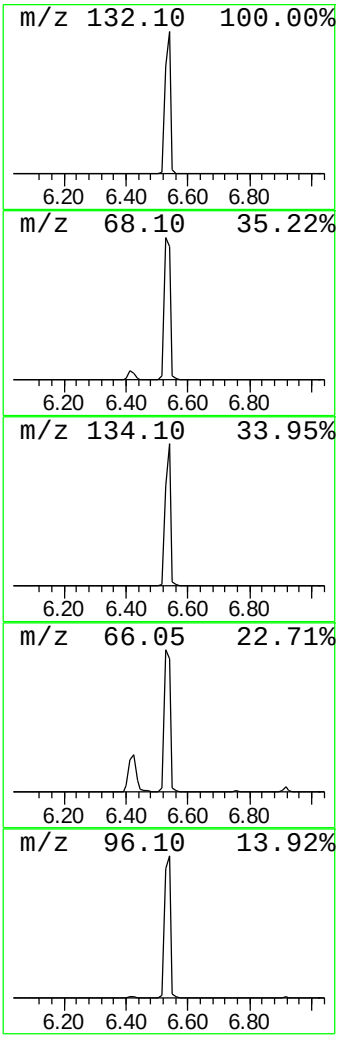
Peak Number 3 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	97.33 ng	5397210	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
ClientSampleId : 39B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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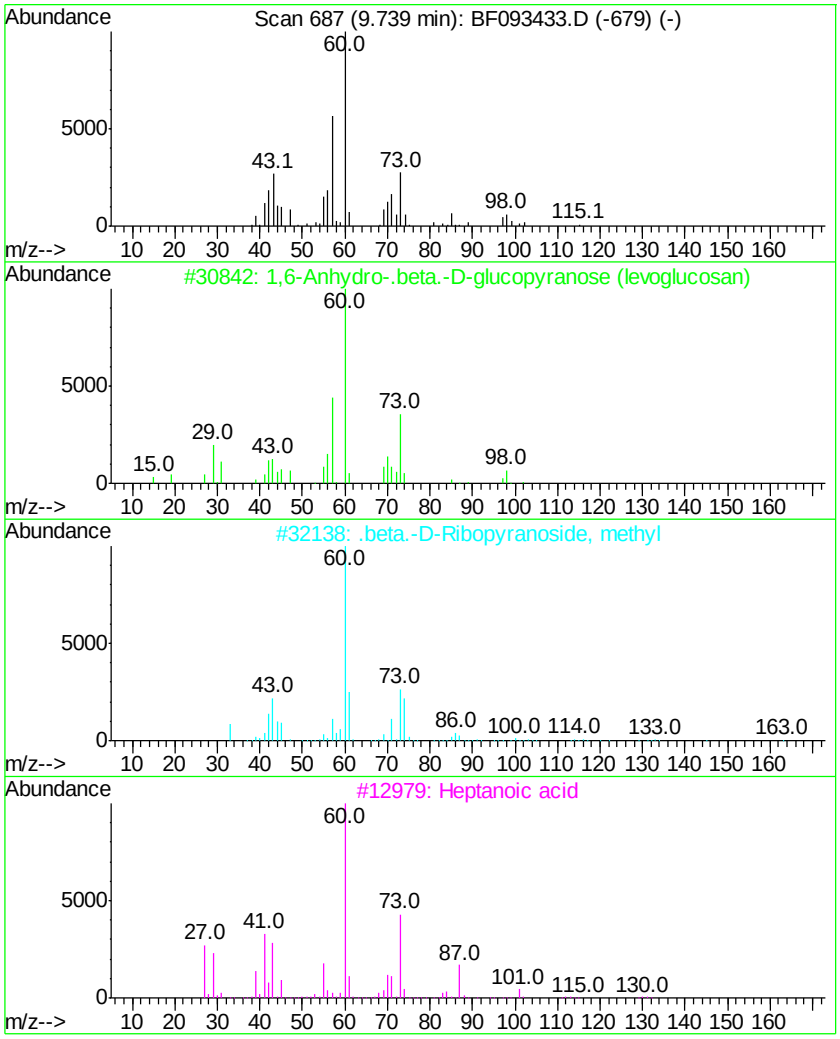
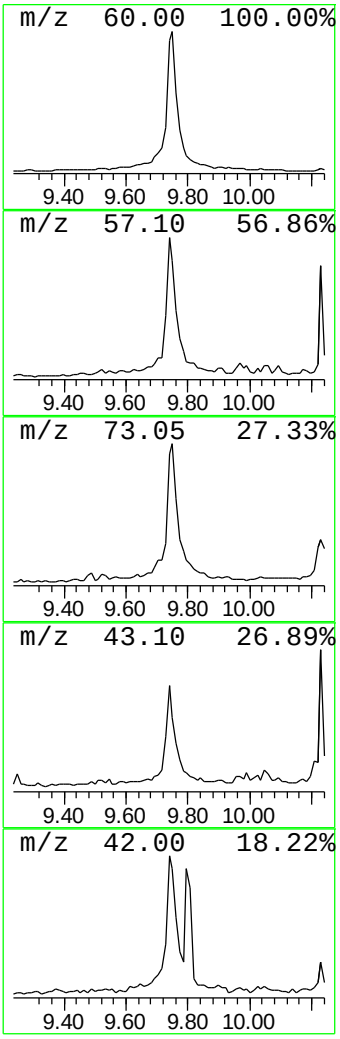
Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	7.14 ng	569306	Acenaphthene-d10	9.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	78
2	.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	53
3	Heptanoic acid	130	C7H14O2	000111-14-8	50
4	Pentanoic acid	102	C5H10O2	000109-52-4	42
5	3,4-Altrosan	162	C6H10O5	1000129-76-4	37





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030817\
Data File : BF093433.D
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Sample : I2099-02
Misc :
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Instrument : BNA_F
ClientSampleId : 39B-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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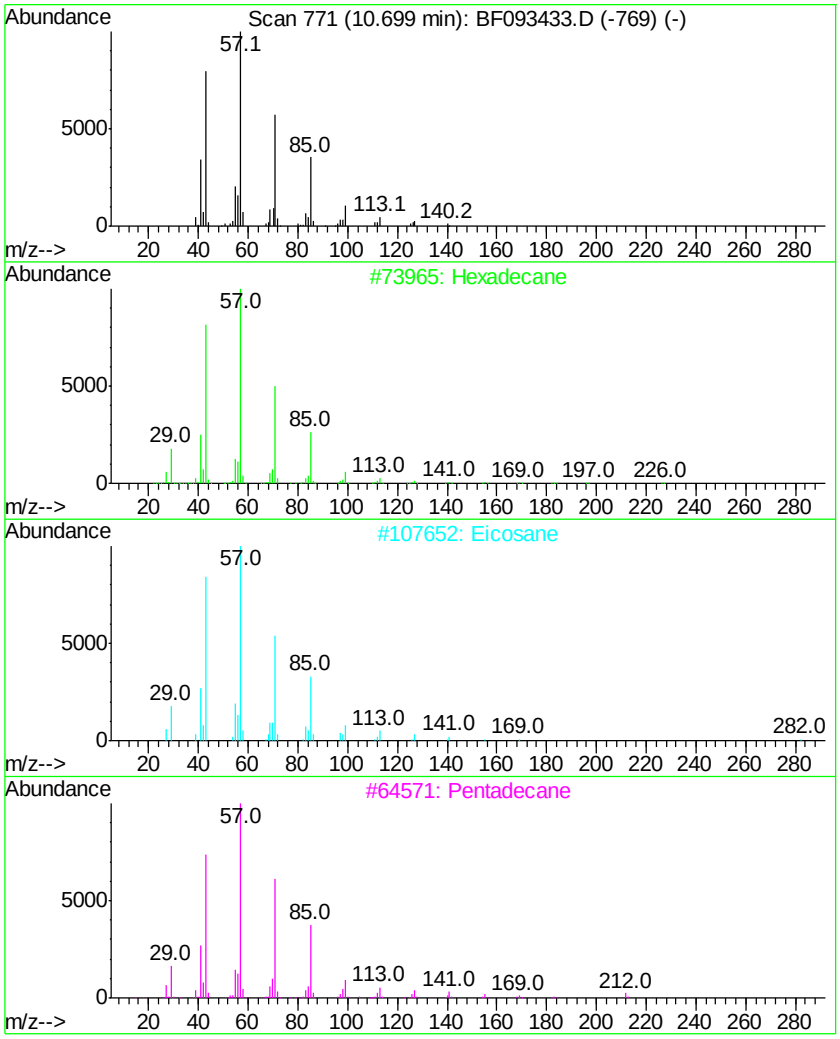
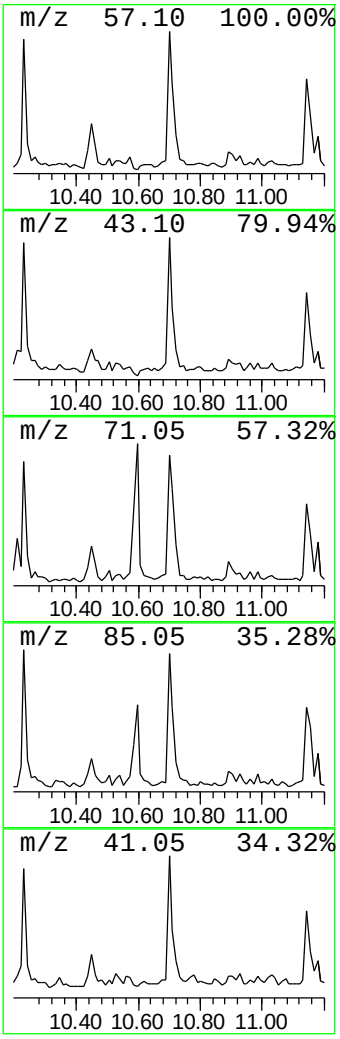
Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.04 ng	168020	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tetradecane	198	C14H30	000629-59-4	83
5	Tridecane	184	C13H28	000629-50-5	78





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TIC Integration Parameters: LSCINT.P

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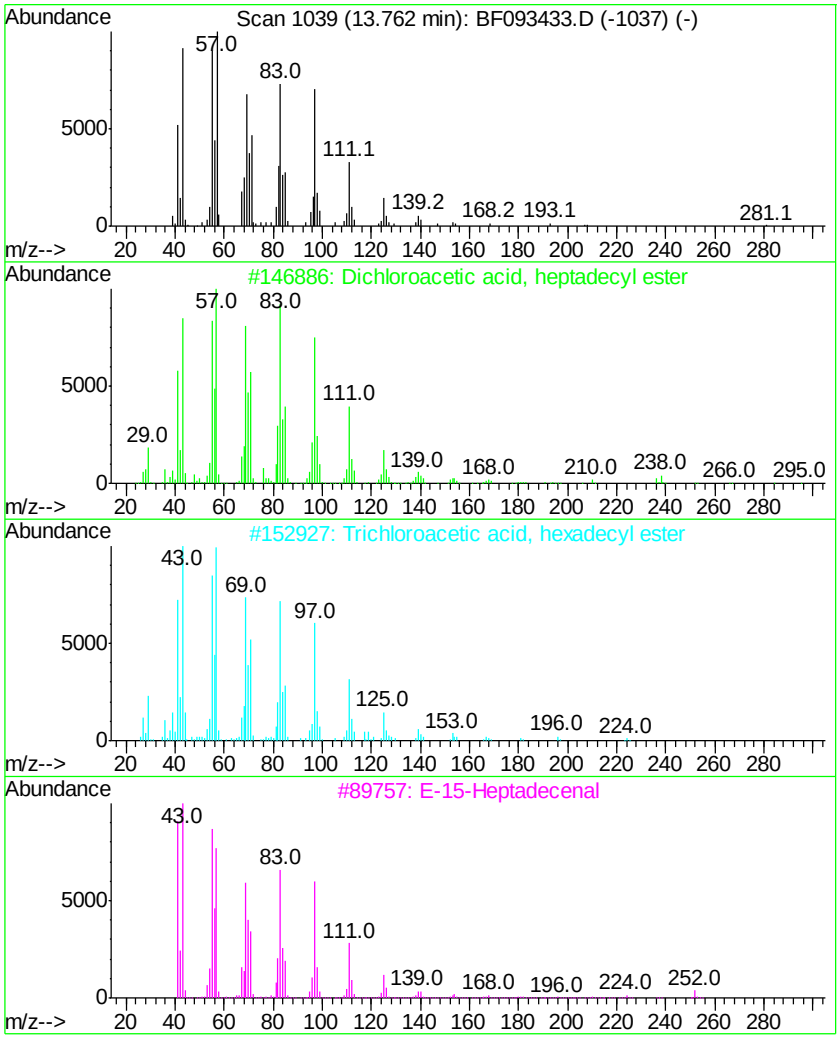
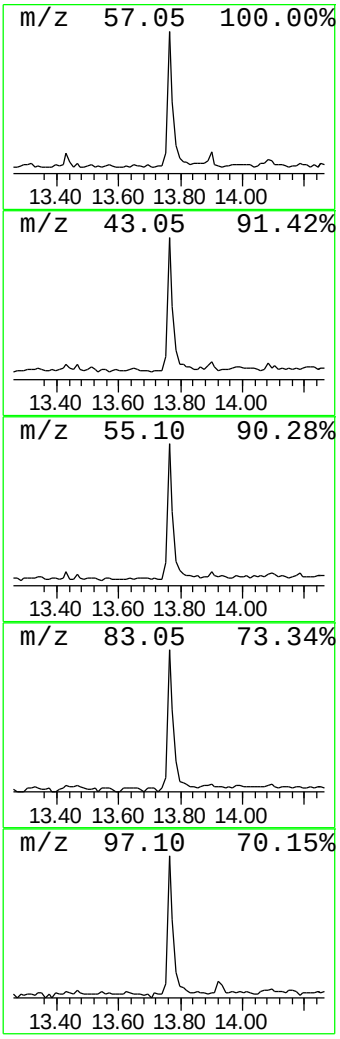
Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	3.83 ng	303309	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91





Tentatively Identified Compound (LSC) summary

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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
Propane, 1,1-dime...	1.96	2.2	ng	121346	1	6.77	1109040	20.0
2-Pentanone, 4-hy...	4.92	24.0	ng	1328400	1	6.77	1109040	20.0
unknown6.54	6.54	97.3	ng	5397210	1	6.77	1109040	20.0
1,6-Anhydro-.beta...	9.74	7.1	ng	569306	3	9.81	1594440	20.0
Hexadecane	10.70	2.0	ng	168020	4	11.28	1643800	20.0
Dichloroacetic ac...	13.76	3.8	ng	303309	5	13.93	1585850	20.0