LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120516\
Data File : BF091442.D
Acq On : 6 Dec 2016 2:26
Operator : UM/SJ
Sample : H5802-06
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

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-BF112916.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	5.030	237	240	243	rBV	519109	605319	12.46%	1.778%
2	5.453	274	277	279	rBV	2383434	2241938	46.13%	6.584%
3	6.481	364	367	369	rBV	1813996	1711554	35.22%	5.027%
4	6.619	376	379	381	rBV	3984456	3702593	76.19%	10.874%
5	6.847	397	399	402	rBV	946388	791499	16.29%	2.325%
6	7.007	410	413	415	rBV	3766103	3368331	69.31%	9.893%
7	7.419	445	449	451	rVB	2542757	3100669	63.80%	9.107%
8	7.510	454	457	459	rBV	46504	64011	1.32%	0.188%
9	8.139	509	512	514	rVB	856633	1053992	21.69%	3.096%
10	9.213	603	606	609	rBV	4758043	4456928	91.71%	13.090%
11	9.887	663	665	667	rBV	1381210	1165694	23.99%	3.424%
12	9.922	667	668	670	rVB	80019	69372	1.43%	0.204%
13	10.676	731	734	737	rBV	2890772	3046259	62.68%	8.947%
14	10.802	743	745	749	rBV	48280	78834	1.62%	0.232%
15	11.248	782	784	785	rVB	59121	51370	1.06%	0.151%
16	11.373	793	795	797	rBV	1308069	1244773	25.61%	3.656%
17	11.911	840	842	846	rVB	407612	486036	10.00%	1.427%
18	12.699	909	911	913	rBV	265144	311315	6.41%	0.914%
19	12.962	931	934	936	rVB	4849509	4859763	100.00%	14.273%
20	13.854	1010	1012	1017	rVB	96260	111223	2.29%	0.327%
21	14.002	1023	1025	1027	rBV	855003	755368	15.54%	2.218%
22	15.431	1147	1150	1153	rBV	638867	772069	15.89%	2.268%

Sum of corrected areas: 34048910

LSC Report - Integrated Chromatogram

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BNA_F
ClientSampleId :
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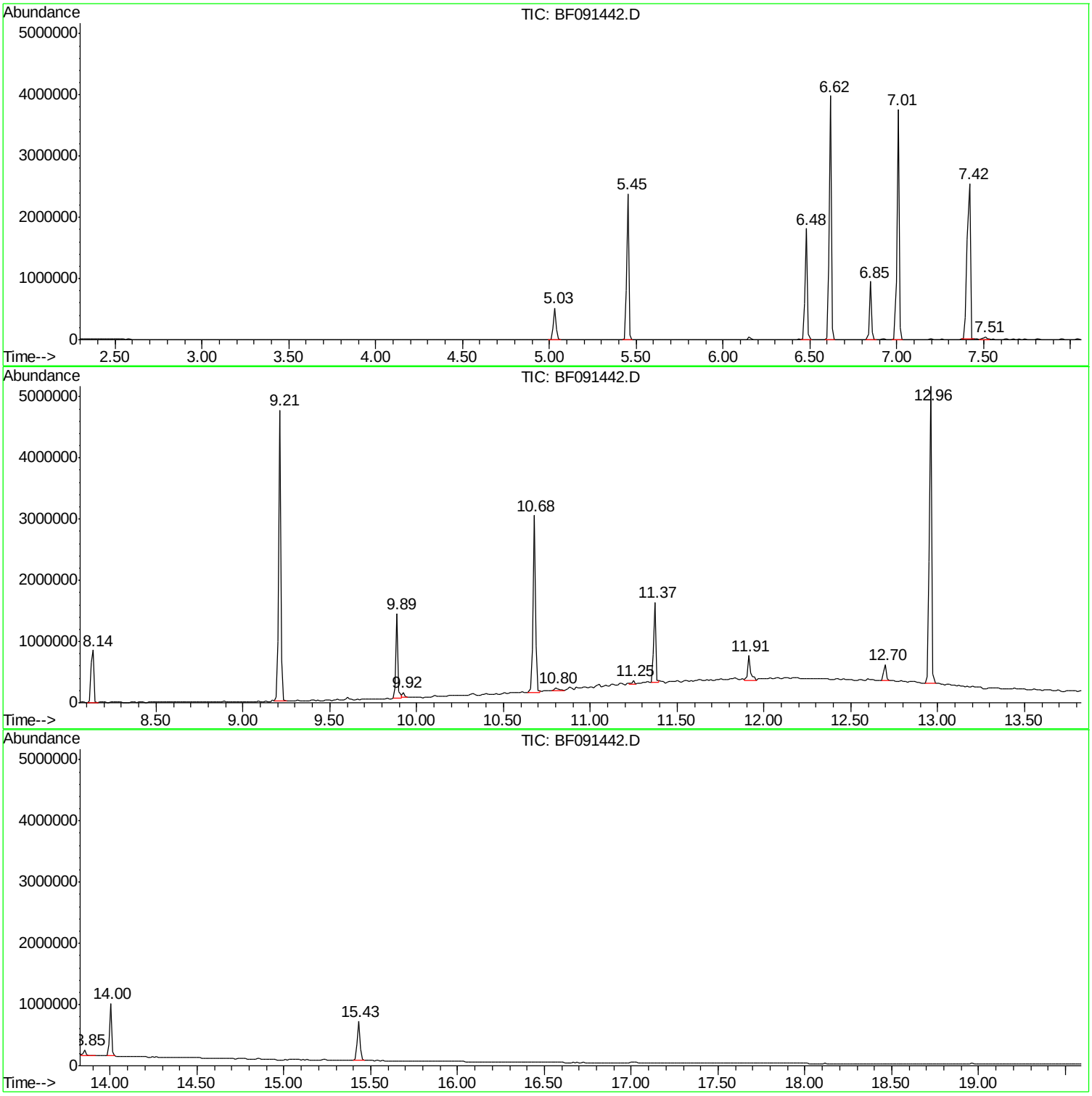
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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TIC Integration Parameters: LSCINT.P

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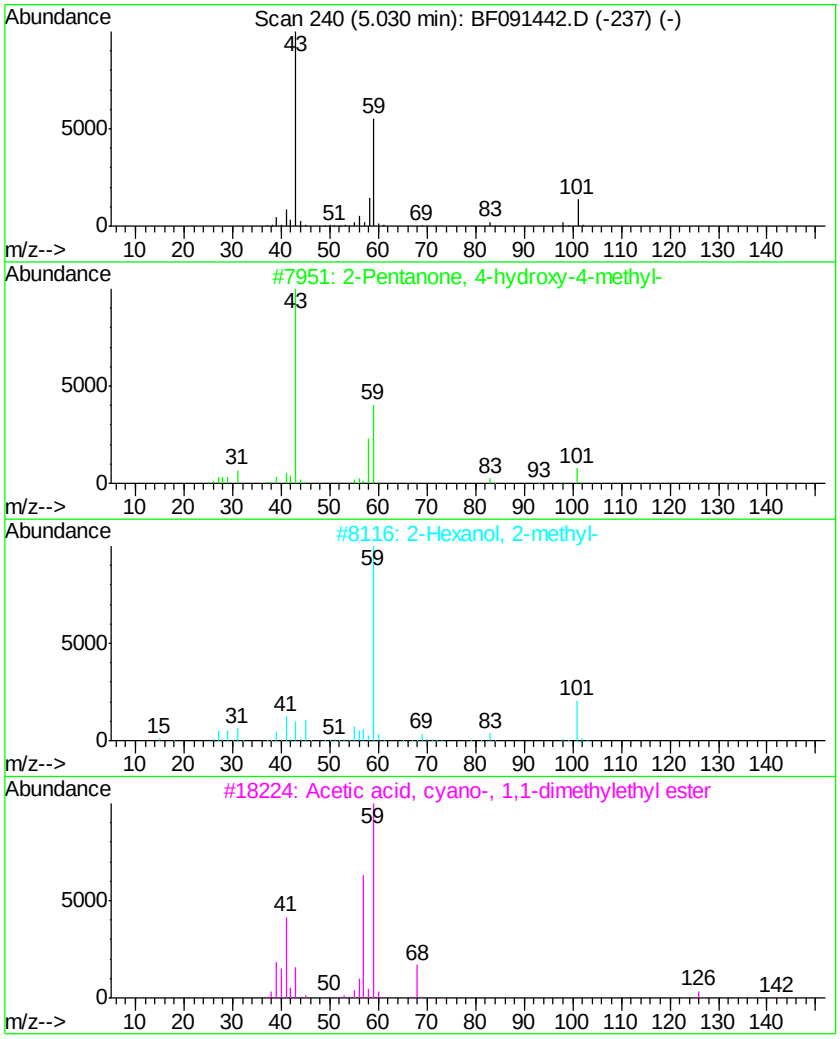
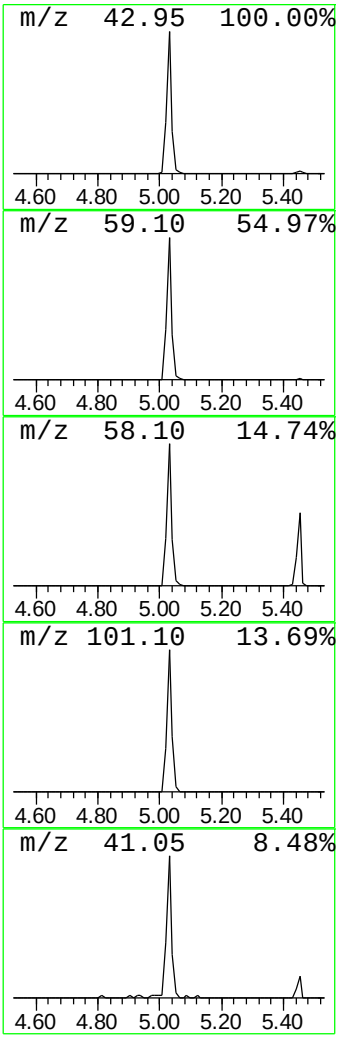
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	15.30 ng	605319	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	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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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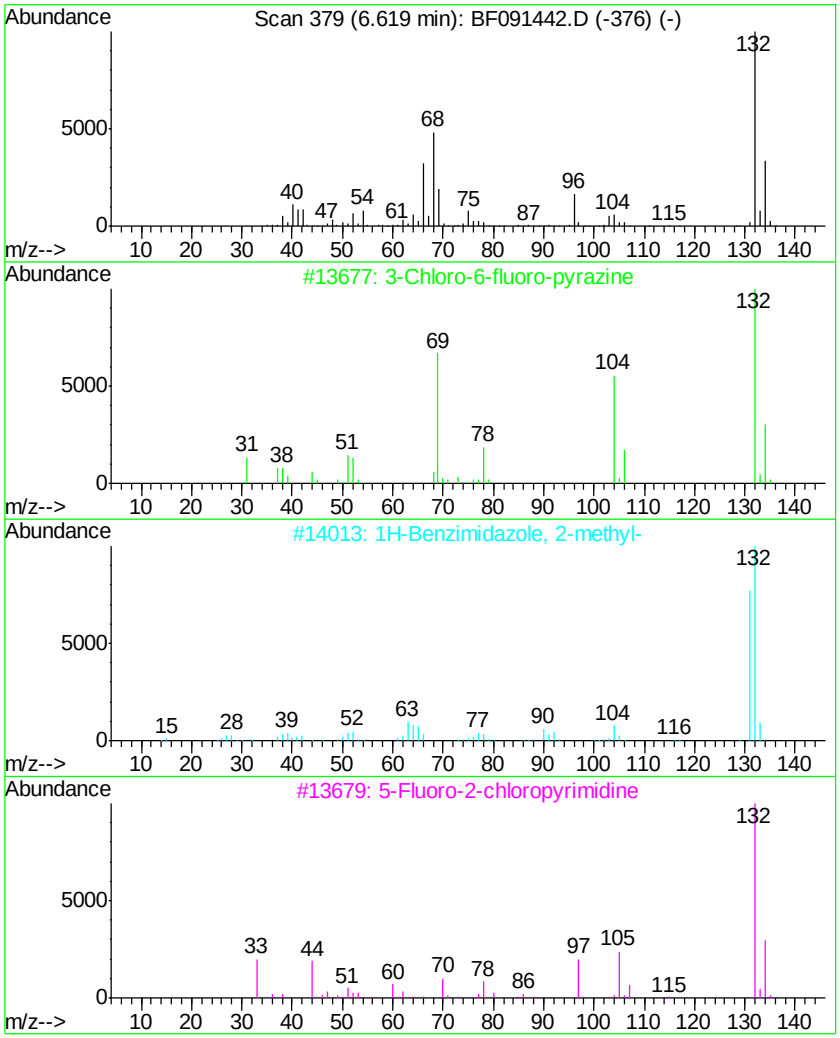
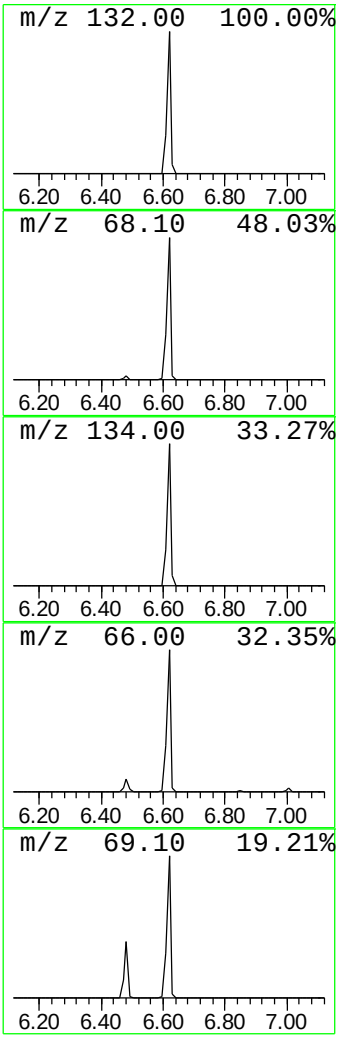
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	93.56 ng	3702590	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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Data File : BF091442.D
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Sample : H5802-06
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
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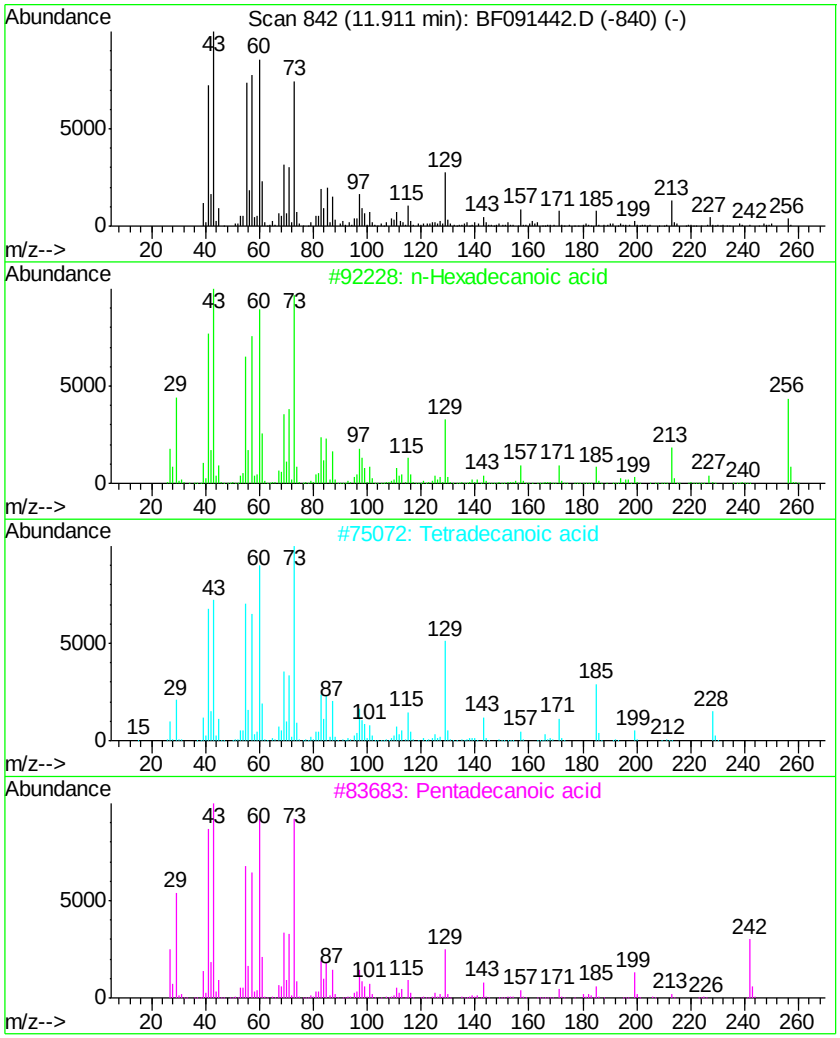
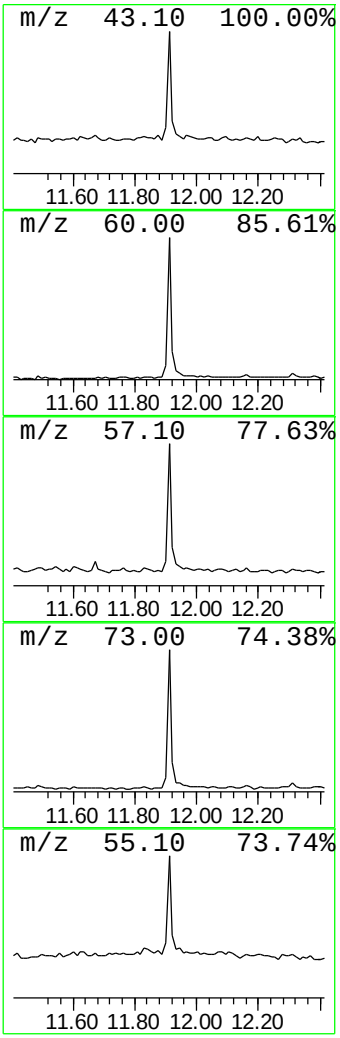
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	7.81 ng	486036	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	68





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Instrument :
BNA_F
ClientSampleId :
MW-05

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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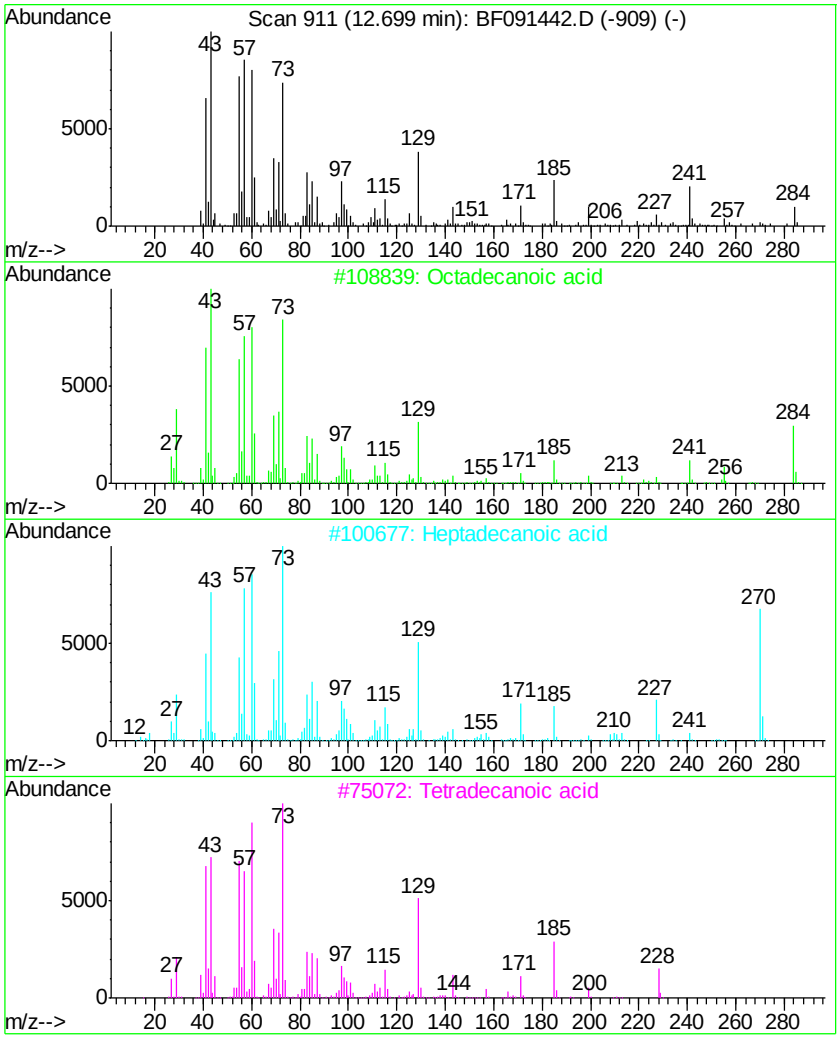
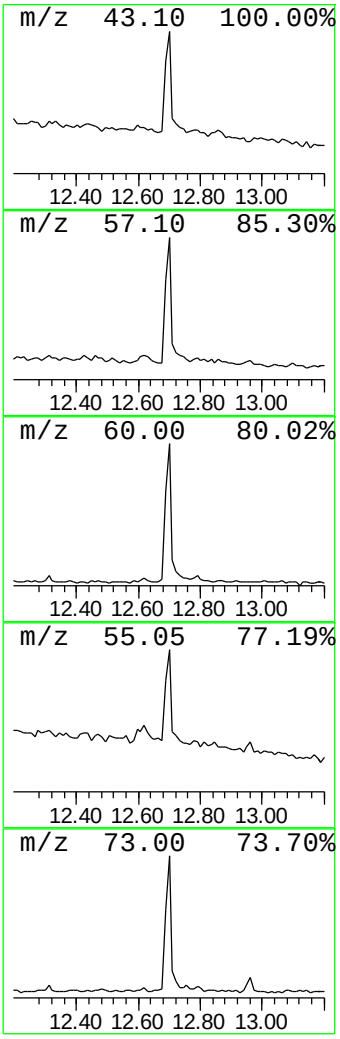
Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	8.24 ng	311315	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	58





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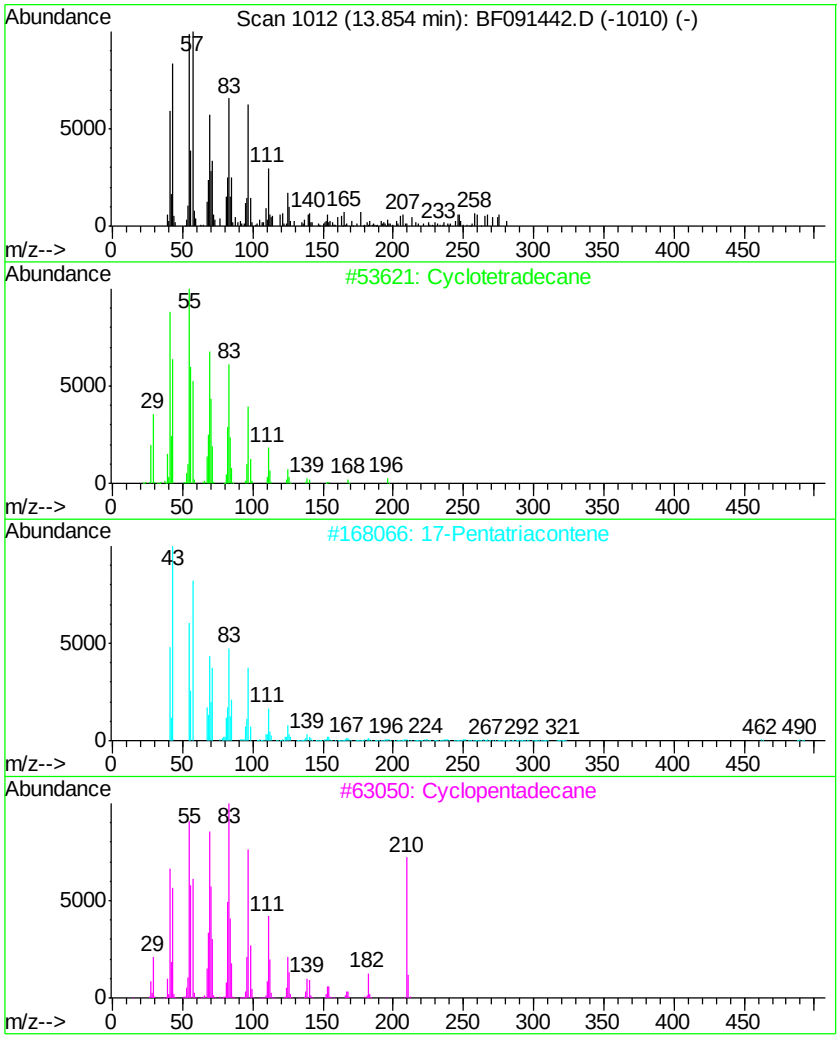
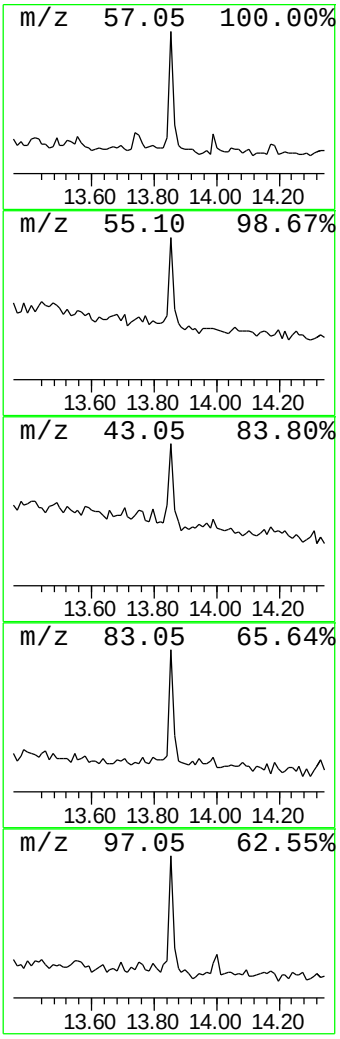
****

Peak Number 6 Cyclotetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.94 ng	111223	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	90
2	17-Pentatriacontene	491	C35H70	006971-40-0	87
3	Cyclopentadecane	210	C15H30	000295-48-7	83
4	1-Hexadecanethiol	258	C16H34S	002917-26-2	72
5	Cyclohexadecane	224	C16H32	000295-65-8	49





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	15.3	ng	605319	1	6.85	791499	20.0
unknown6.62	6.62	93.6	ng	3702590	1	6.85	791499	20.0
n-Hexadecanoic acid	11.91	7.8	ng	486036	4	11.37	1244770	20.0
Octadecanoic acid	12.70	8.2	ng	311315	5	14.00	755368	20.0
Cyclotetradecane	13.85	2.9	ng	111223	5	14.00	755368	20.0