LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093648.D
Acq On : 14 Mar 2017 10:19
Operator : SJ/MA
Sample : I2201-24
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-127

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	2.458	48	50	61	rBV	47514	154598	2.58%	0.300%
2	4.173	197	200	205	rVB	44543	81583	1.36%	0.158%
3	4.424	219	222	229	rVB2	29072	74765	1.25%	0.145%
4	4.882	259	262	290	rVB	1116816	2544953	42.40%	4.939%
5	5.316	298	300	320	rBV	4153875	5989639	99.79%	11.624%
6	5.716	333	335	347	rVB	72369	146329	2.44%	0.284%
7	6.367	391	392	400	rBV	3223102	5514107	91.86%	10.701%
8	6.482	400	402	405	rVB	4819346	5191287	86.49%	10.074%
9	6.710	420	422	430	rVB	1088577	1161969	19.36%	2.255%
10	6.859	433	435	438	rBV	3749644	4154429	69.21%	8.062%
11	7.282	470	472	487	rBV	2874930	3963367	66.03%	7.692%
12	8.002	533	535	549	rBV	1390322	1593894	26.55%	3.093%
13	9.076	626	629	632	rBV	4290670	6002449	100.00%	11.649%
14	9.751	686	688	691	rBV	1278090	1738818	28.97%	3.374%
15	10.551	756	758	761	rBV2	2474774	3204946	53.39%	6.220%
16	11.248	817	819	825	rBV	1719942	1734754	28.90%	3.367%
17	12.654	939	942	944	rBV	213310	179725	2.99%	0.349%
18	12.837	955	958	961	rBV	4762027	5272192	87.83%	10.232%
19	13.362	1002	1004	1006	rBV	98950	117722	1.96%	0.228%
20	13.888	1048	1050	1060	rVB	1015473	1533579	25.55%	2.976%
21	15.294	1170	1173	1186	rBV	673133	1173905	19.56%	2.278%

Sum of corrected areas: 51529010

LSC Report - Integrated Chromatogram

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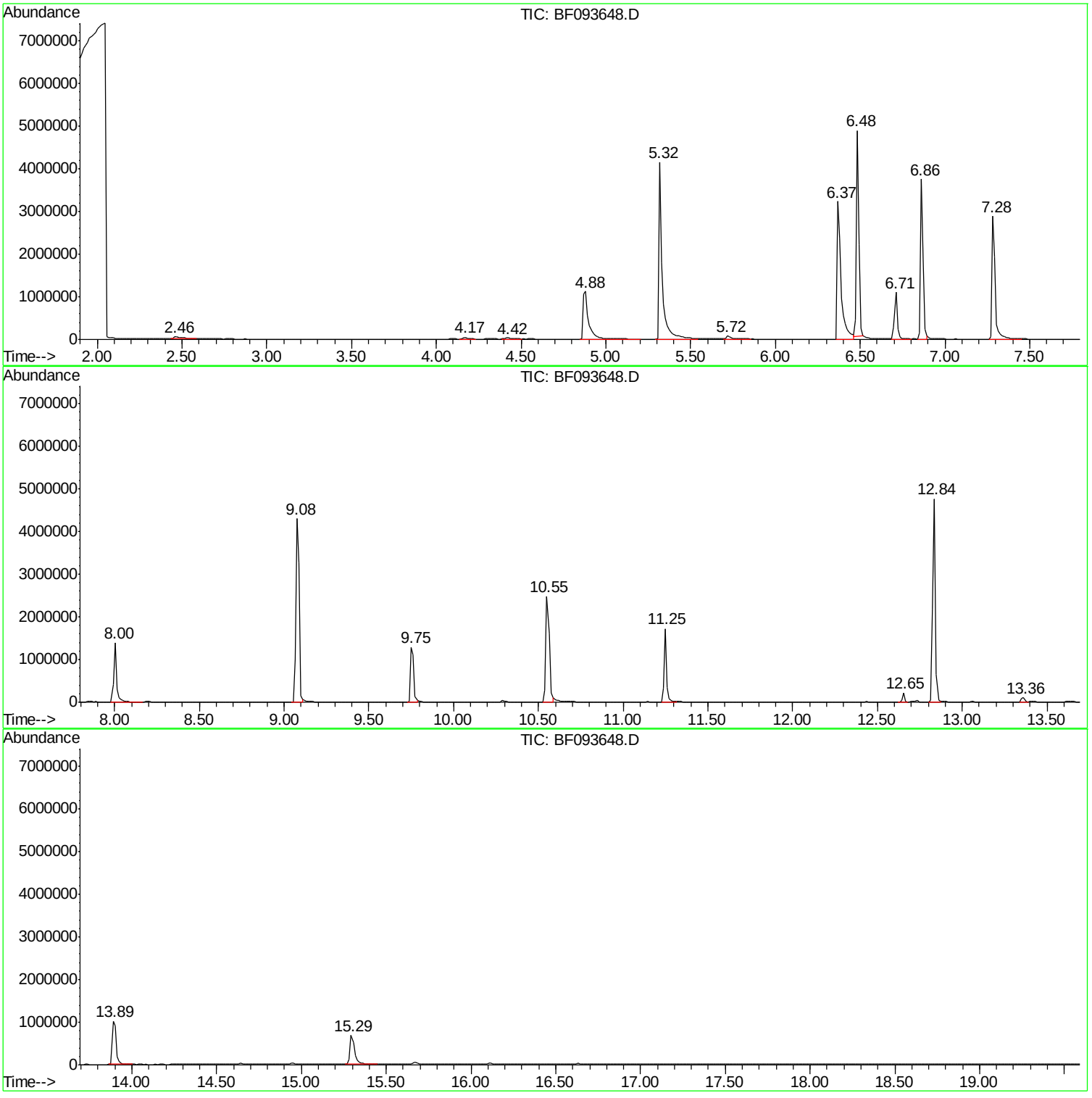
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-127

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



Library Search Compound Report

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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
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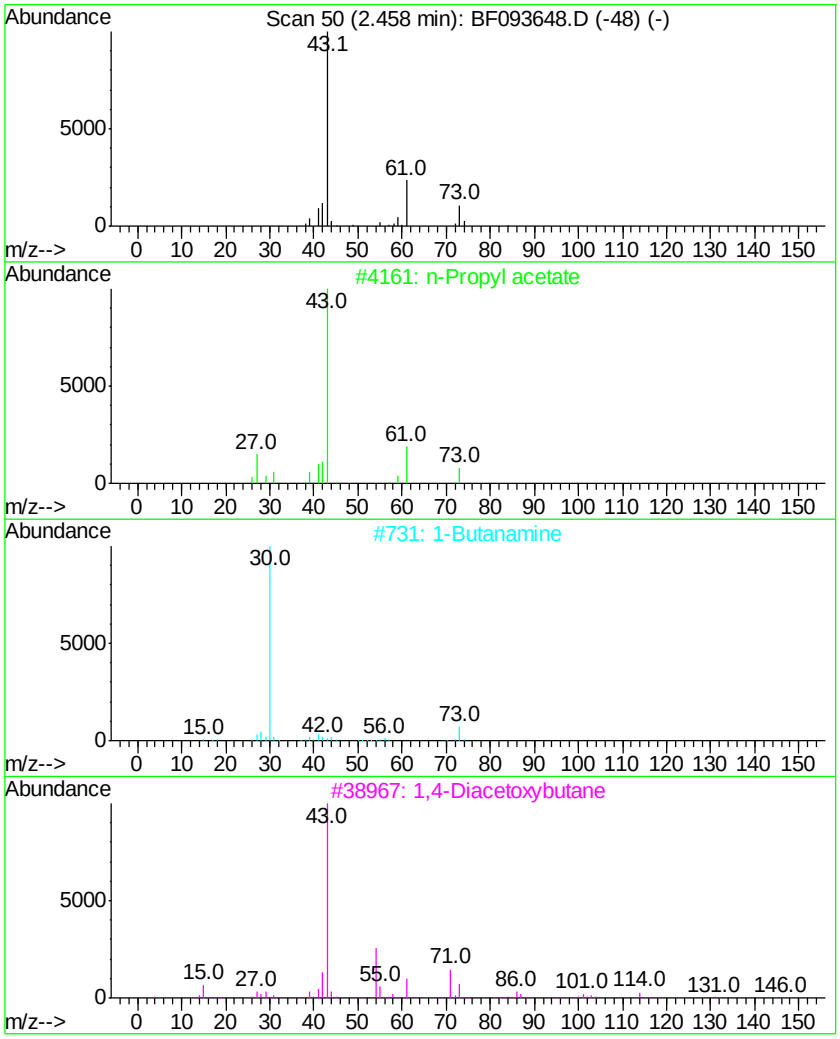
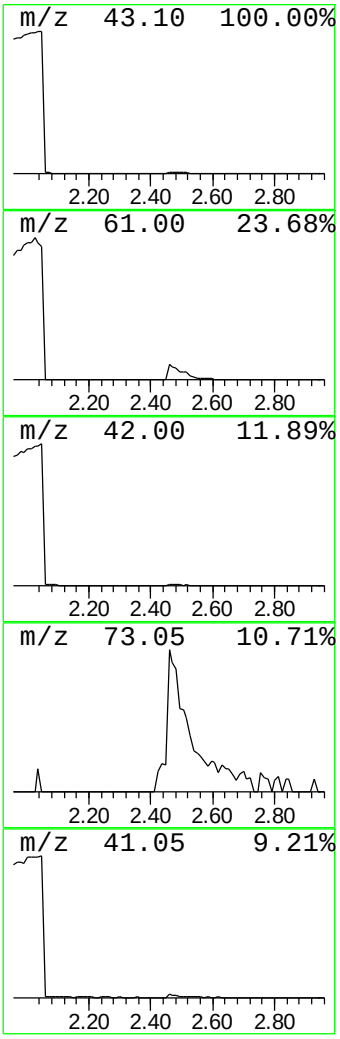
Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.46	2.66 ng	154598	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	72
2	1-Butanamine	73	C4H11N	000109-73-9	9
3	1,4-Diacetoxybutane	174	C8H14O4	033934-62-2	9
4	Sulfurous acid, dipropyl ester	166	C6H14O3S	000623-98-3	9
5	Isobutylamine	73	C4H11N	000078-81-9	5





Library Search Compound Report

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Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-127

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TIC Library : C:\DATABASE\NIST02.L
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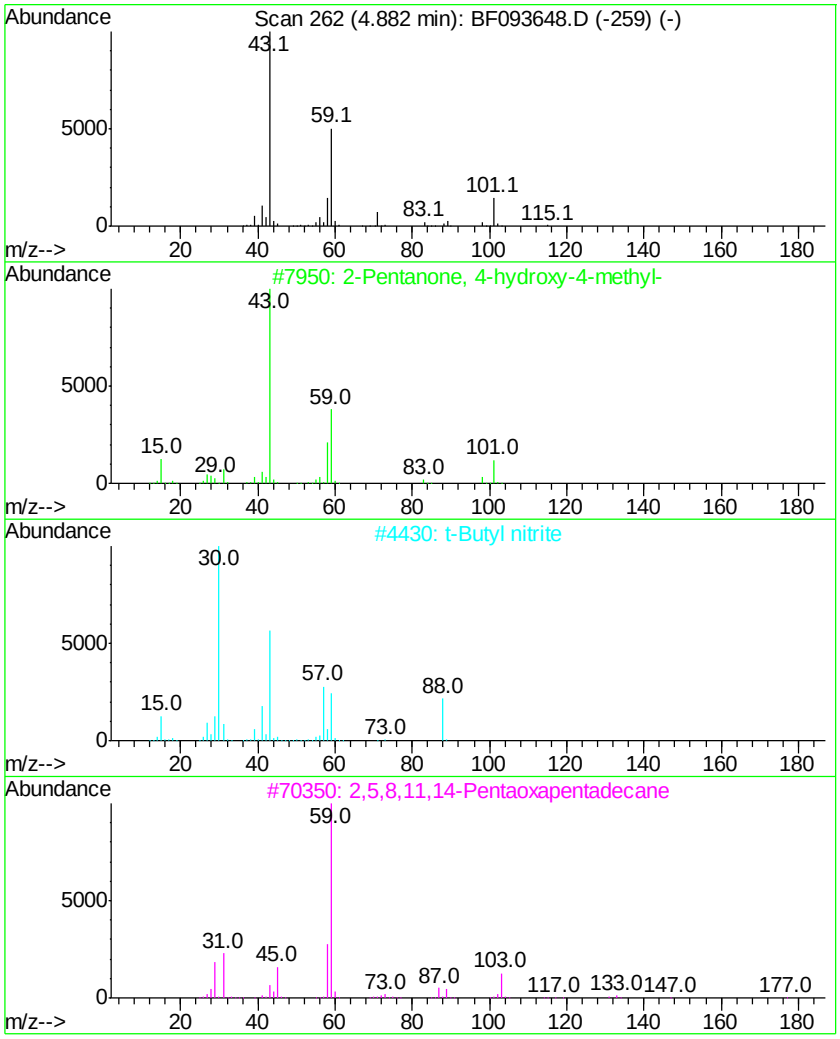
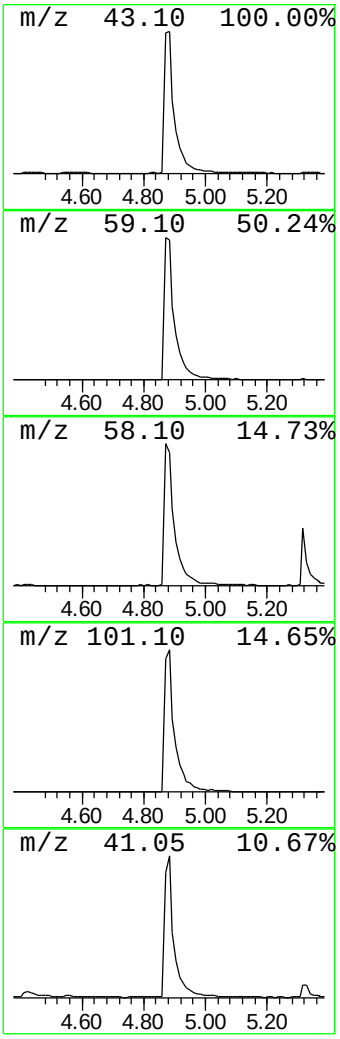
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	43.80 ng	2544950	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	38
3	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	28
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	25





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Misc :
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Instrument : BNA_F
ClientSampleId : D-127

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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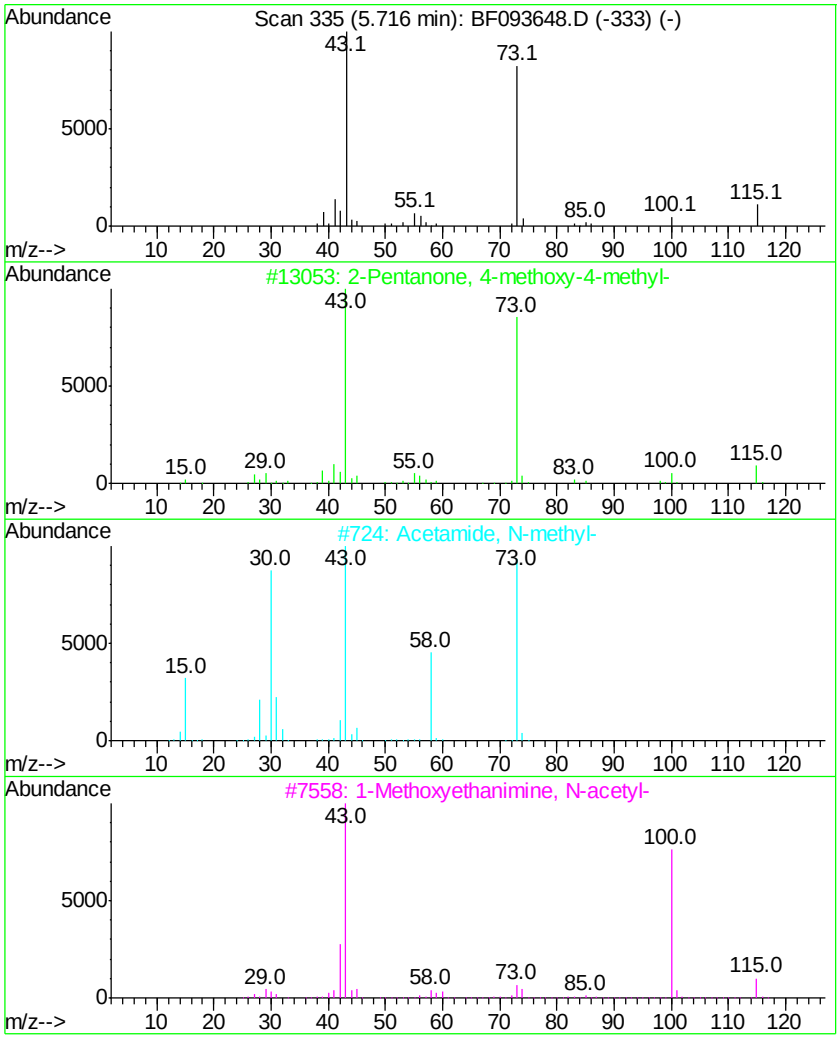
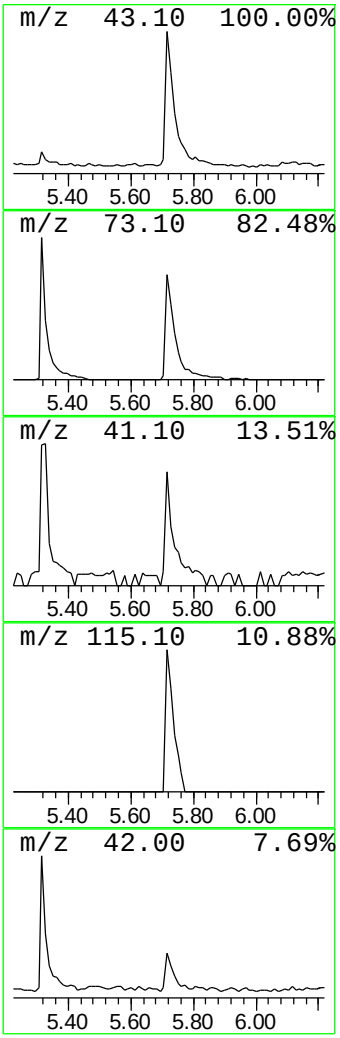
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.52 ng	146329	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	47
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
4	Hexane, 2-methyl-	100	C7H16	000591-76-4	10
5	Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	9





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Instrument : BNA_F
ClientSampleId : D-127

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TIC Library : C:\DATABASE\NIST02.L
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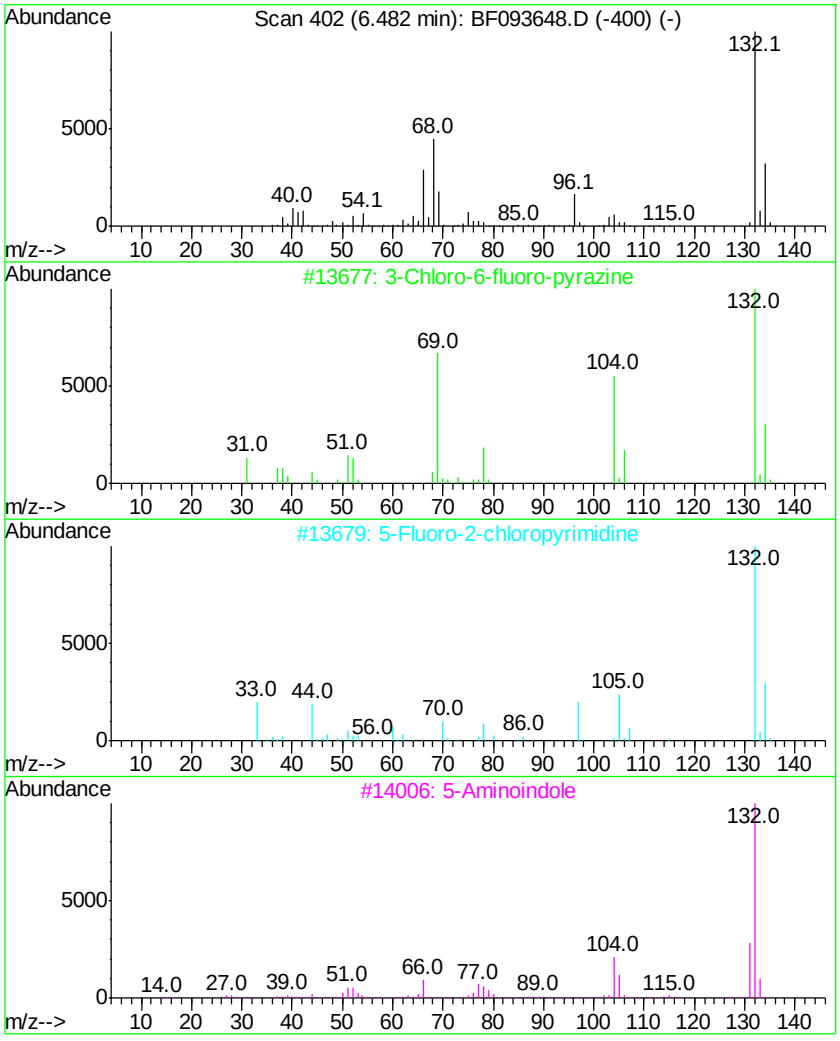
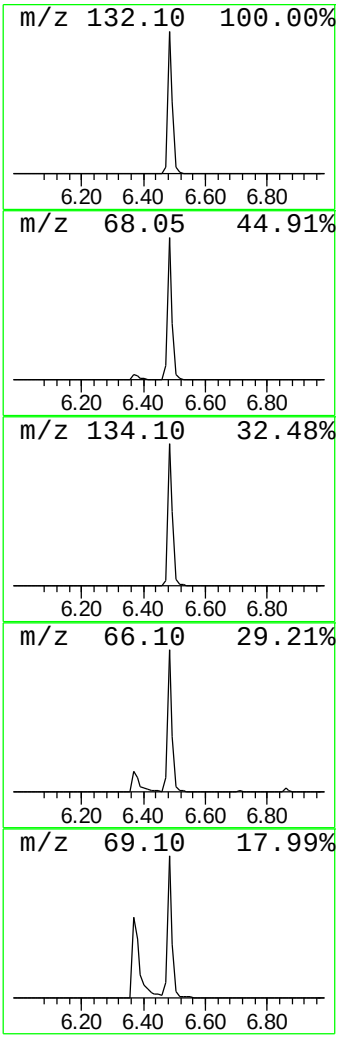
Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	89.35 ng	5191290	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
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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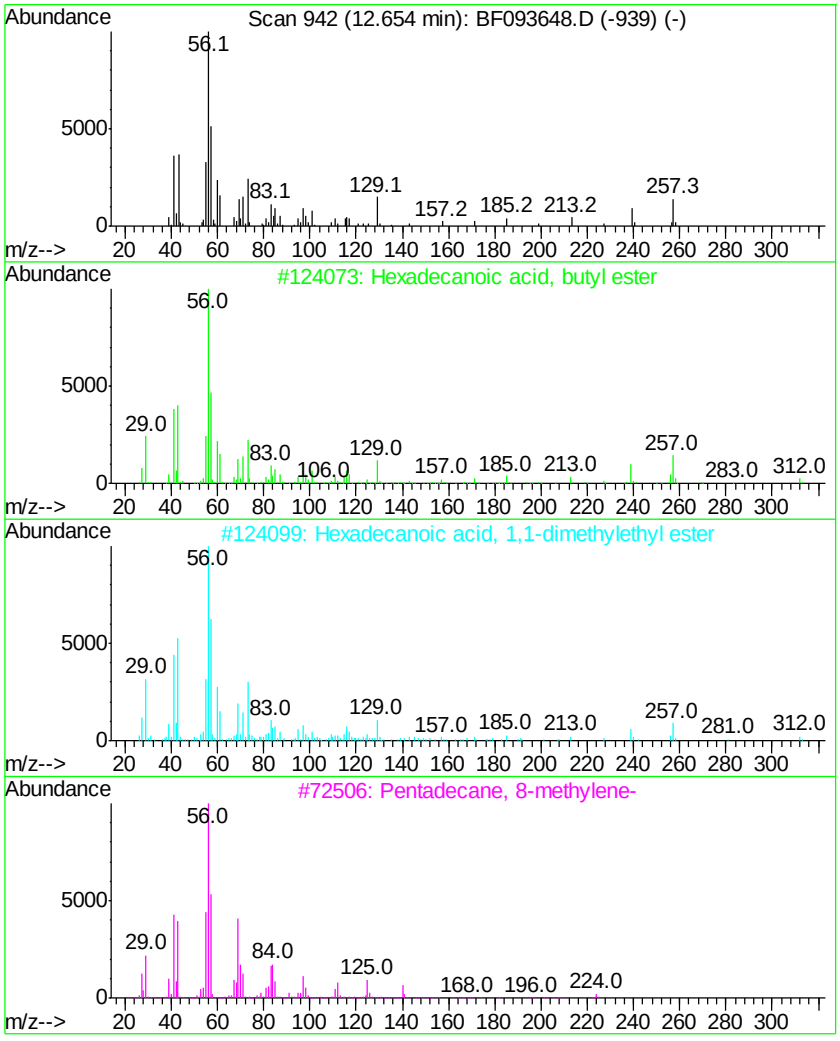
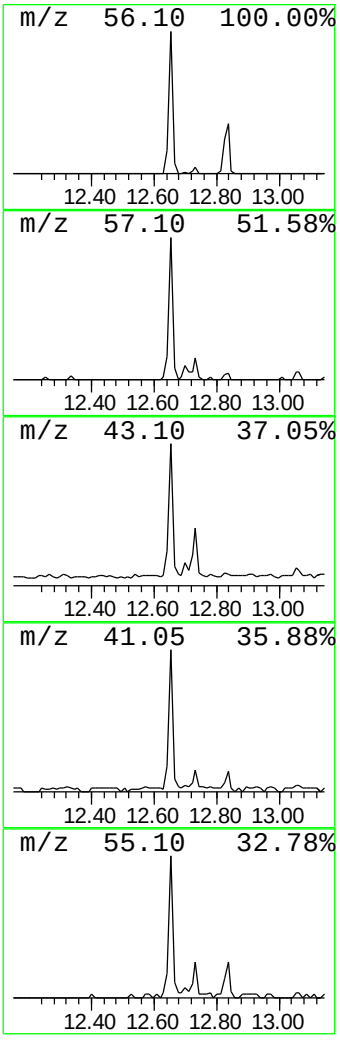
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.34 ng	179725	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	68
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	43
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38





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
n-Propyl acetate	2.46	2.7	ng	154598	1	6.71	1161970	20.0
2-Pentanone, 4-hy...	4.88	43.8	ng	2544950	1	6.71	1161970	20.0
2-Pentanone, 4-me...	5.72	2.5	ng	146329	1	6.71	1161970	20.0
unknown6.48	6.48	89.3	ng	5191290	1	6.71	1161970	20.0
Hexadecanoic acid...	12.65	2.3	ng	179725	5	13.90	1533580	20.0