LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100419.D
Acq On : 11 Nov 2017 4:22
Operator : SJ/JU
Sample : I6355-09
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110317-TIFR-F-U-M

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-BF110817.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	2.210	17	21	30	rVB	82060	117375	2.58%	0.422%
2	5.122	512	516	522	rBV	279318	290576	6.39%	1.044%
3	5.516	579	583	586	rBV	1853908	1637068	36.01%	5.881%
4	6.516	749	753	756	rBV	1289606	1065814	23.44%	3.829%
5	6.545	756	758	763	rVB	65718	54571	1.20%	0.196%
6	6.669	774	779	782	rBV	2891520	2697530	59.33%	9.691%
7	6.904	815	819	822	rBV	999953	920660	20.25%	3.307%
8	7.063	841	846	849	rBV	3270786	3301353	72.61%	11.860%
9	7.469	909	915	918	rBV	2591092	2866680	63.05%	10.298%
10	8.180	1032	1036	1040	rBV	1302306	1122370	24.69%	4.032%
11	8.733	1126	1130	1134	rBV	81207	63478	1.40%	0.228%
12	9.263	1214	1220	1223	rBV	4376398	4546739	100.00%	16.334%
13	9.939	1329	1335	1346	rVB	1221254	1140683	25.09%	4.098%
14	10.604	1445	1448	1451	rVB	84001	60670	1.33%	0.218%
15	10.651	1452	1456	1459	rBV	274594	242577	5.34%	0.871%
16	10.721	1464	1468	1472	rBV	1638872	1611027	35.43%	5.787%
17	11.421	1583	1587	1591	rVB	1066786	911058	20.04%	3.273%
18	12.821	1822	1825	1830	rVB	169916	130309	2.87%	0.468%
19	12.898	1830	1838	1842	rBV5	36940	53973	1.19%	0.194%
20	13.010	1852	1857	1860	rBV	3471067	3442955	75.72%	12.368%
21	13.527	1942	1945	1948	rBV	108501	86657	1.91%	0.311%
22	14.062	2032	2036	2039	rBV	907883	828198	18.22%	2.975%
23	15.545	2282	2288	2295	rBV	461582	644324	14.17%	2.315%

Sum of corrected areas: 27836645

LSC Report - Integrated Chromatogram

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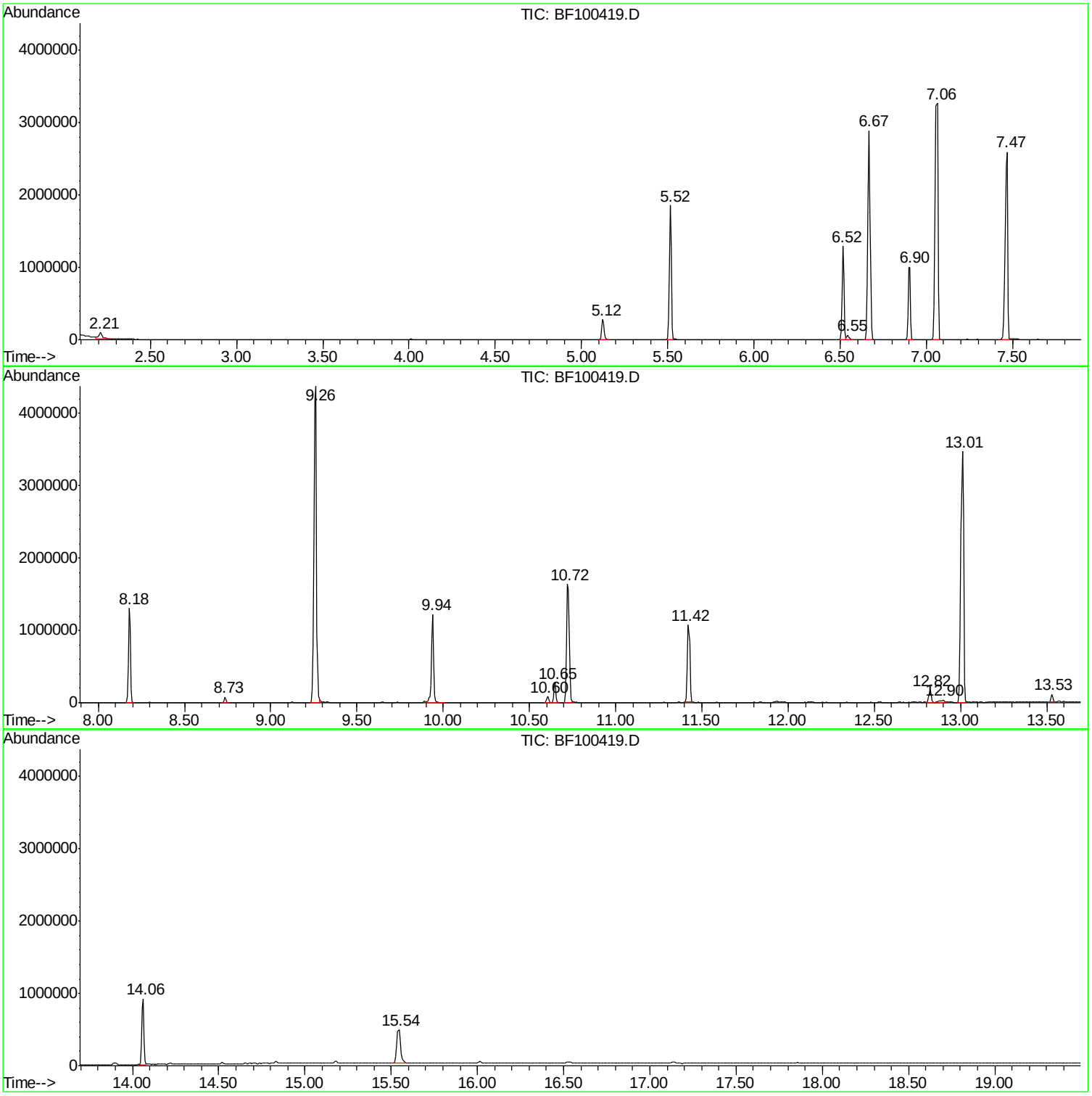
Sample : I6355-09
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110317-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF100419.D
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Operator : SJ/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : 110317-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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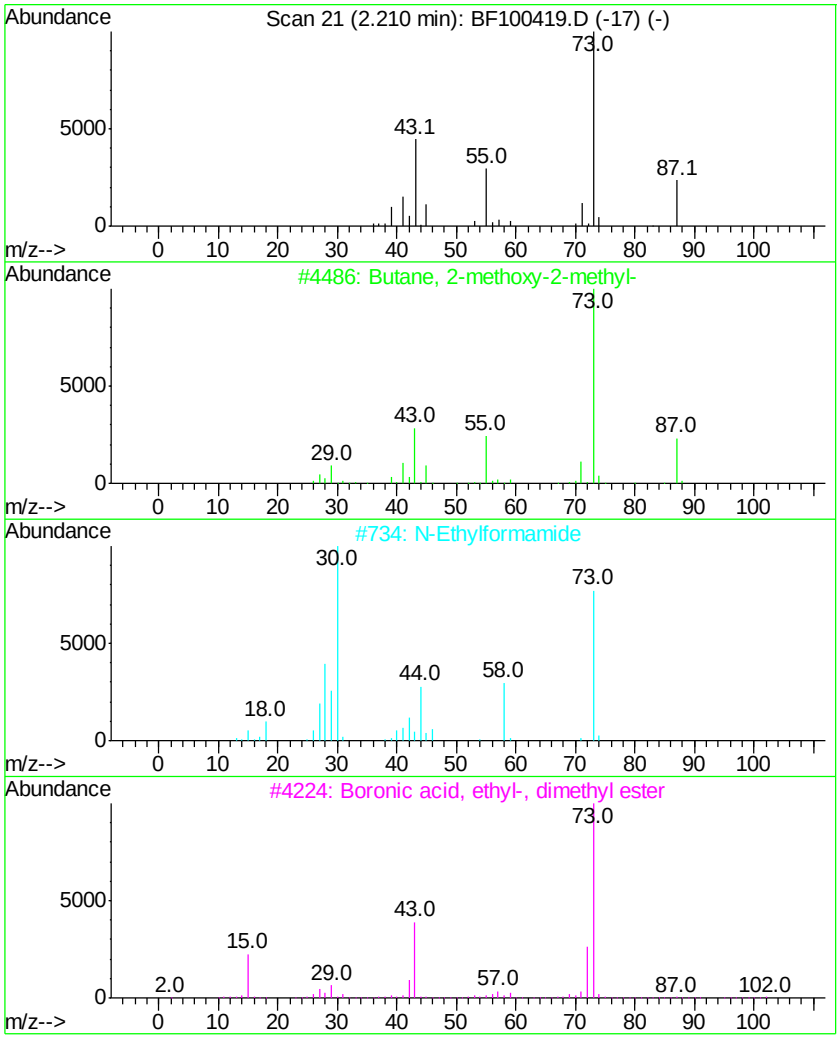
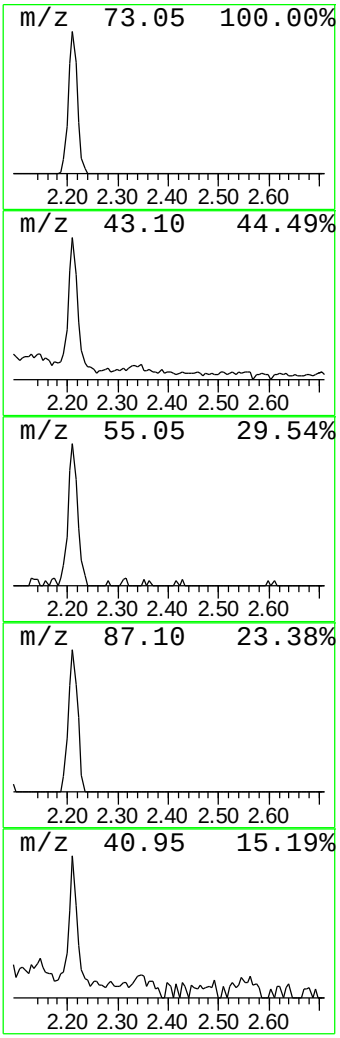
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	2.55 ng	117375	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110317-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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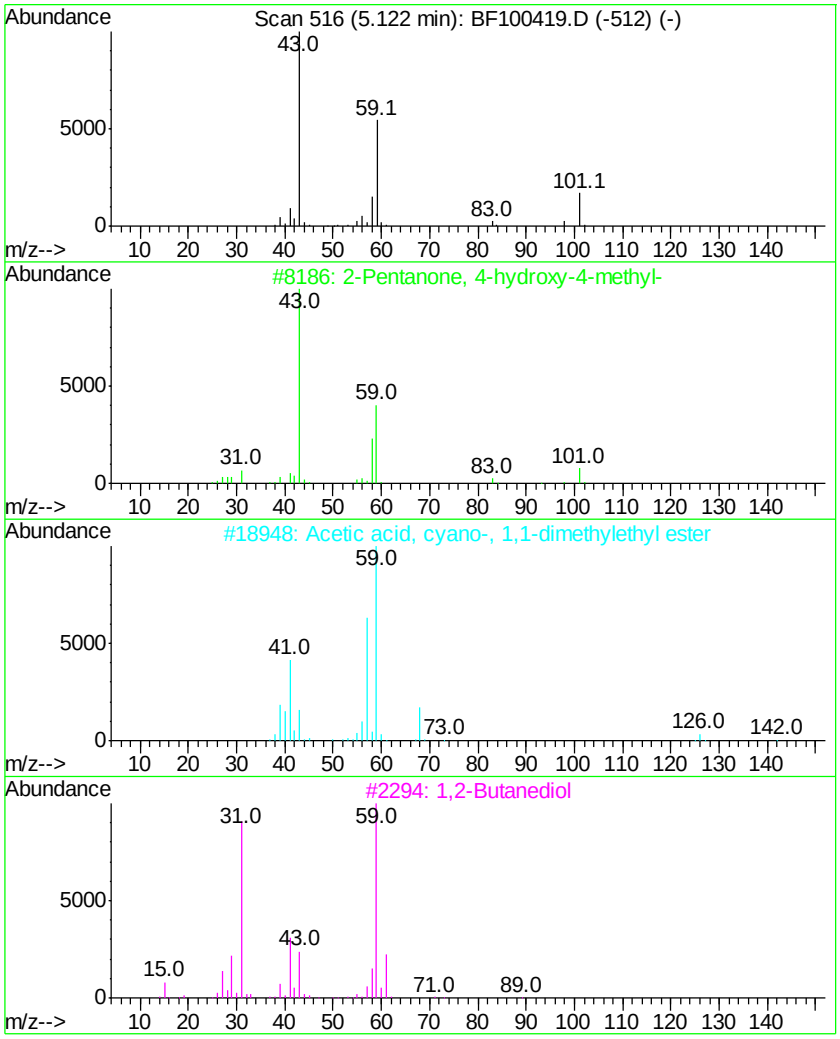
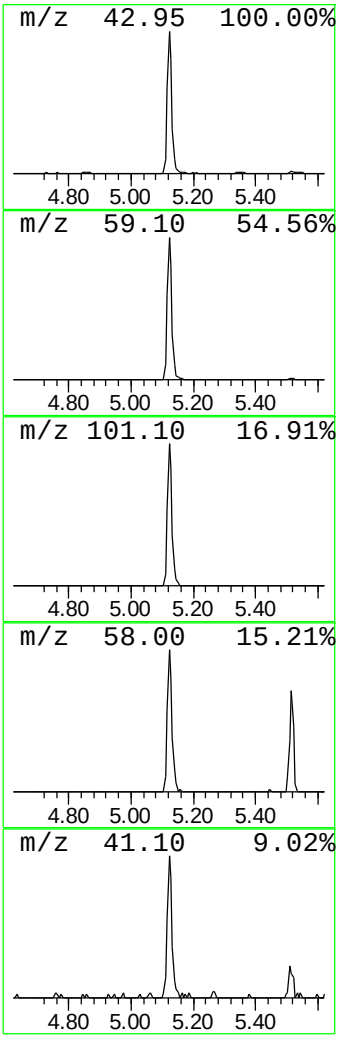
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.31 ng	290576	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	1,2-Butanediol	90	C4H10O2	000584-03-2	9
4	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Operator : SJ/JU
Sample : I6355-09
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110317-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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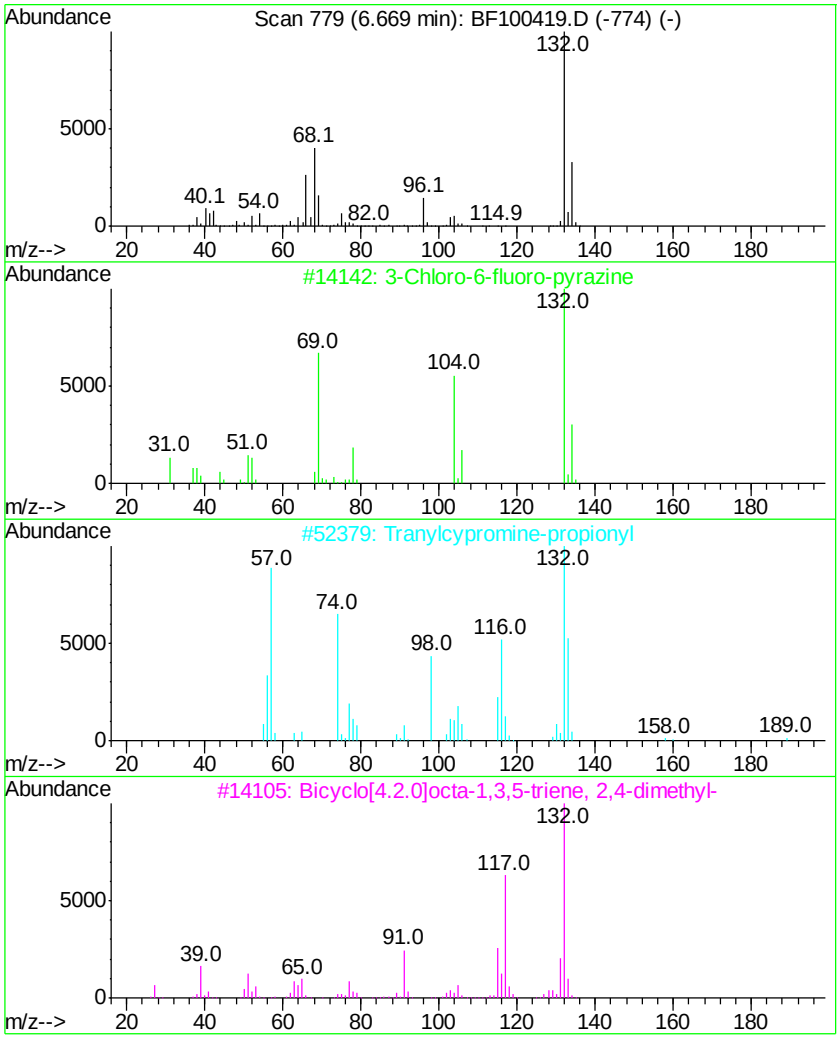
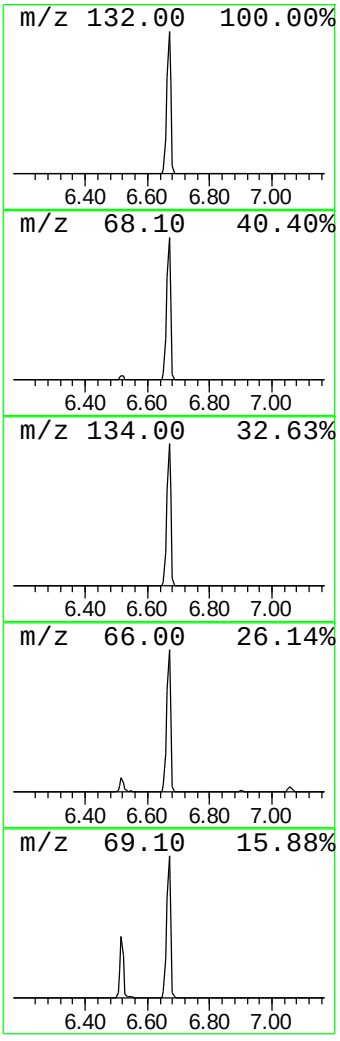
Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	58.60 ng	2697530	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : 110317-TIFR-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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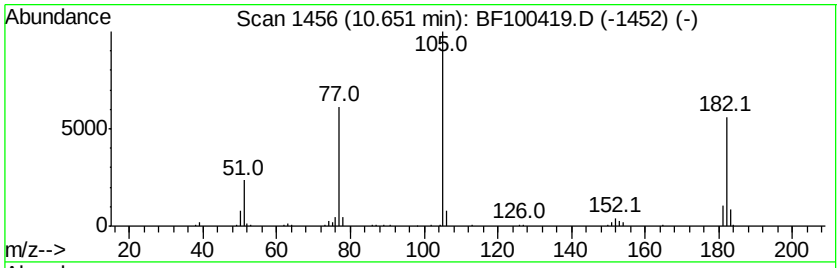
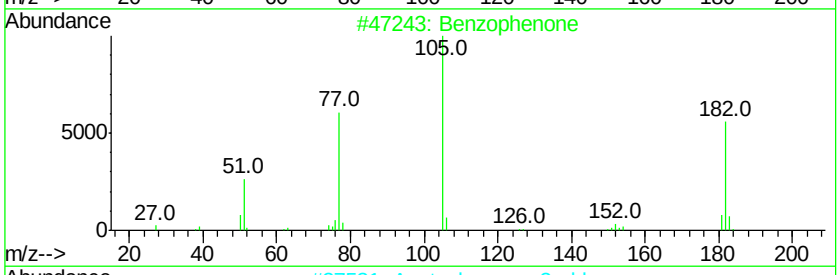
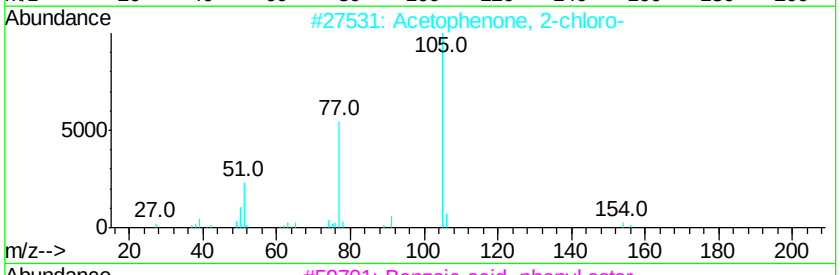
Peak Number 5 Benzophenone Concentration Rank 4

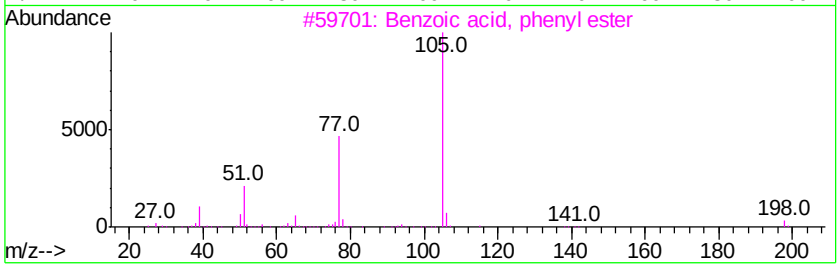
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	4.25 ng	242577	Acenaphthene-d10	9.94

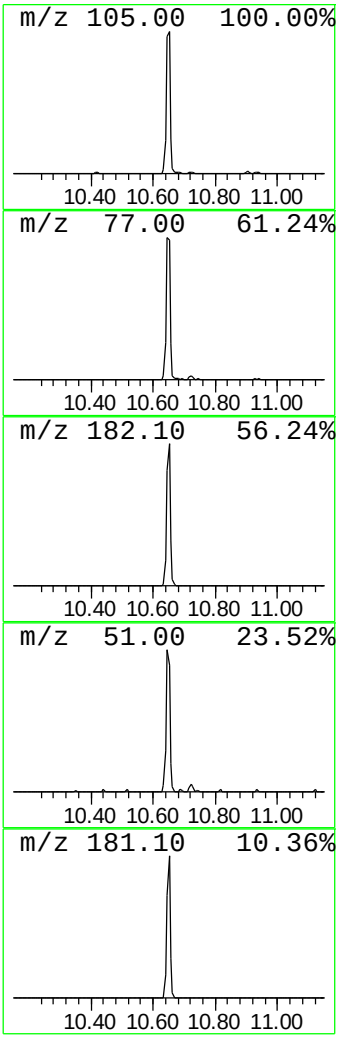
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47











Library Search Compound Report

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

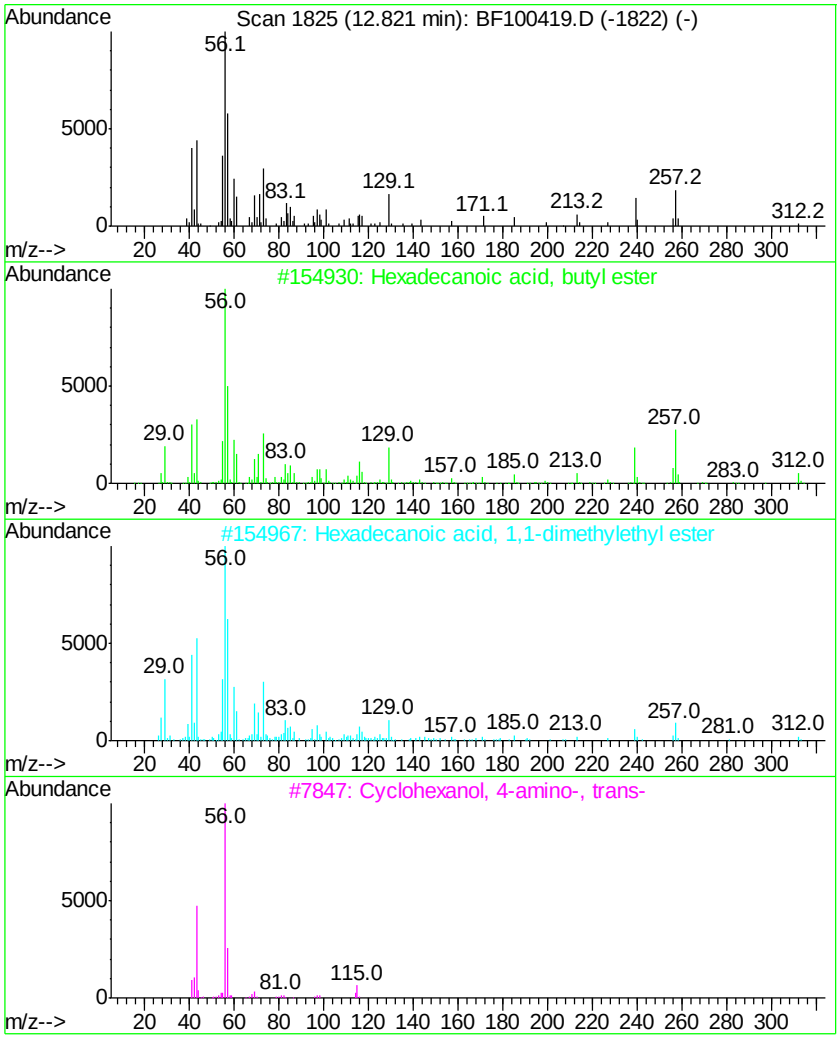
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

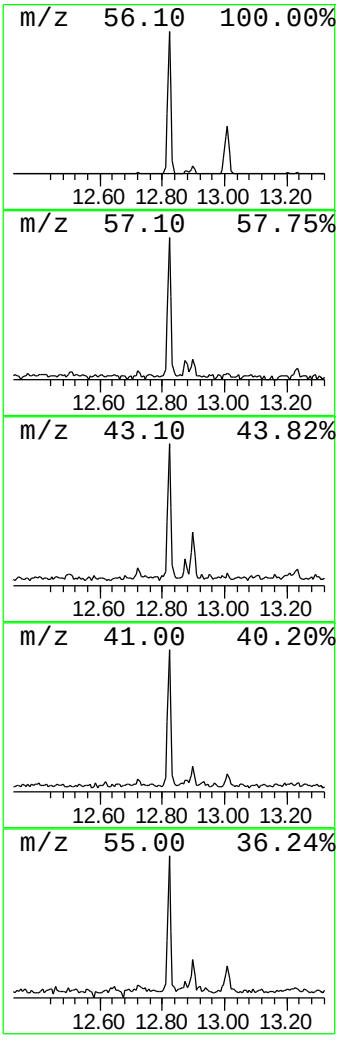
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	3.15 ng	130309	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	64
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	55
3	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
4	Cyclohexanamine	99	C6H13N	000108-91-8	38
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38





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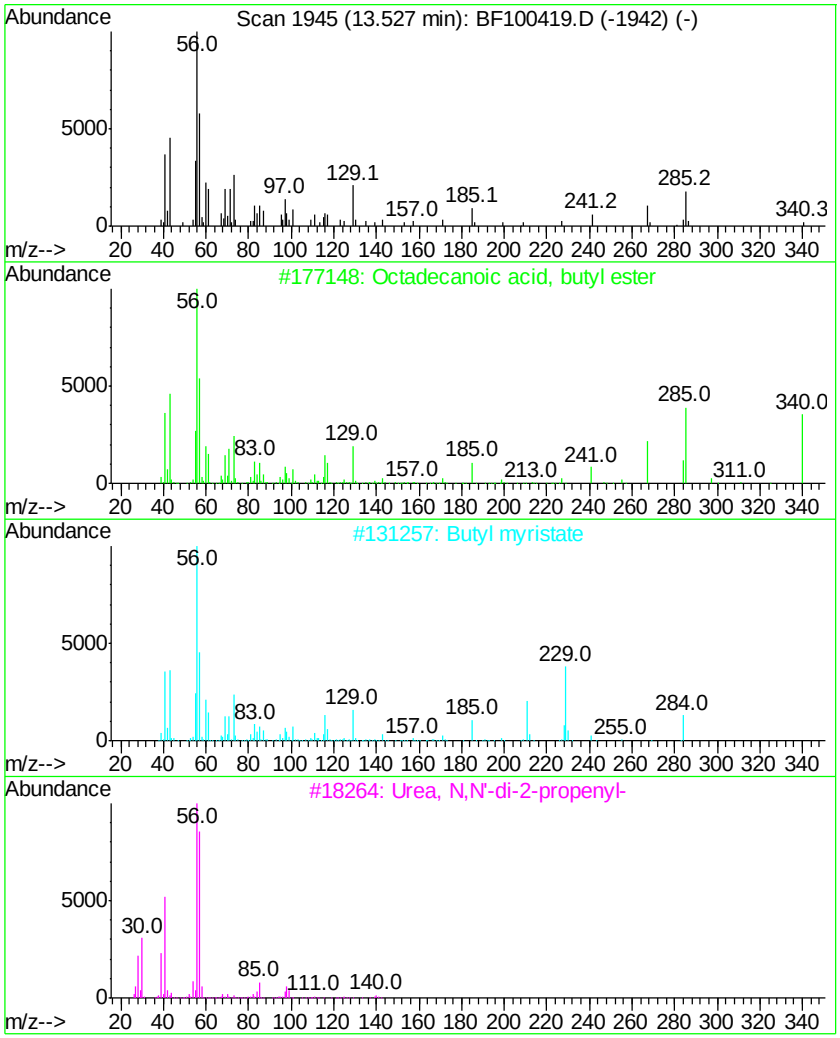
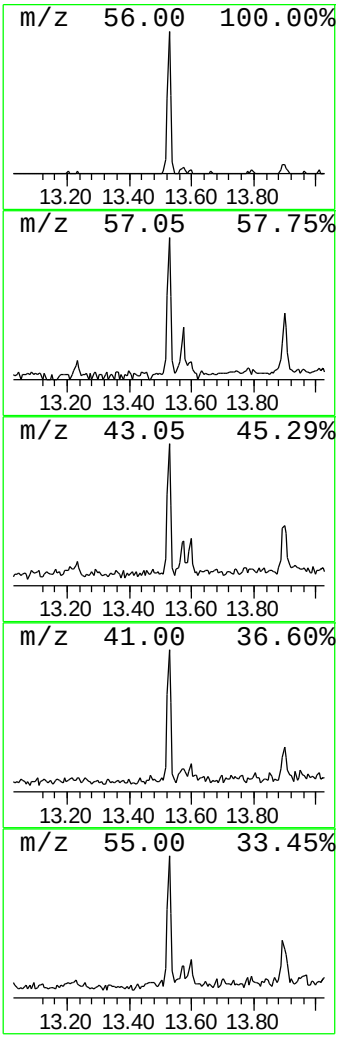
****

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.09 ng	86657	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2	Butyl myristate	284	C18H36O2	000110-36-1	80
3	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	32





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
Butane, 2-methoxy...	2.21	2.5	ng	117375	1	6.90	920660	20.0
2-Pentanone, 4-hy...	5.12	6.3	ng	290576	1	6.90	920660	20.0
unknown6.67	6.67	58.6	ng	2697530	1	6.90	920660	20.0
Benzophenone	10.65	4.3	ng	242577	3	9.94	1140680	20.0
Hexadecanoic acid...	12.82	3.1	ng	130309	5	14.06	828198	20.0
Octadecanoic acid...	13.53	2.1	ng	86657	5	14.06	828198	20.0