LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100418.D
Acq On : 11 Nov 2017 3:55
Operator : SJ/JU
Sample : I6355-08
Misc :
ALS Vial : 36 Sample Multiplier: 1

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

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	2.204	16	20	29	rVB2	68679	100389	2.26%	0.372%
2	5.122	513	516	522	rBV	288109	295205	6.64%	1.095%
3	5.516	579	583	586	rBV	1801506	1576775	35.44%	5.847%
4	6.516	749	753	756	rBV	1269577	1062612	23.89%	3.940%
5	6.545	756	758	765	rVB	68345	57765	1.30%	0.214%
6	6.669	774	779	782	rBV	2905385	2579507	57.98%	9.565%
7	6.904	815	819	822	rVB	959391	882829	19.85%	3.273%
8	7.063	841	846	849	rVB	3246388	3217973	72.34%	11.932%
9	7.469	909	915	918	rBV	2641944	2789017	62.69%	10.342%
10	8.180	1032	1036	1040	rBV	1247381	1081090	24.30%	4.009%
11	9.263	1214	1220	1223	rBV	4272026	4448582	100.00%	16.495%
12	9.939	1329	1335	1349	rVB	1201159	1106456	24.87%	4.103%
13	10.604	1445	1448	1452	rVB	84649	61100	1.37%	0.227%
14	10.645	1452	1455	1459	rBV	120186	109106	2.45%	0.405%
15	10.721	1464	1468	1472	rBV	1574638	1568306	35.25%	5.815%
16	11.421	1584	1587	1591	rBV	1059638	920729	20.70%	3.414%
17	12.821	1822	1825	1828	rBV	169485	130141	2.93%	0.483%
18	12.898	1830	1838	1842	rVB4	38548	56914	1.28%	0.211%
19	13.010	1852	1857	1860	rBV	3447227	3409571	76.64%	12.642%
20	13.527	1942	1945	1948	rBV	110429	86160	1.94%	0.319%
21	14.062	2032	2036	2042	rVB	885641	791350	17.79%	2.934%
22	15.545	2283	2288	2301	rVB	457529	637567	14.33%	2.364%

Sum of corrected areas: 26969144

LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
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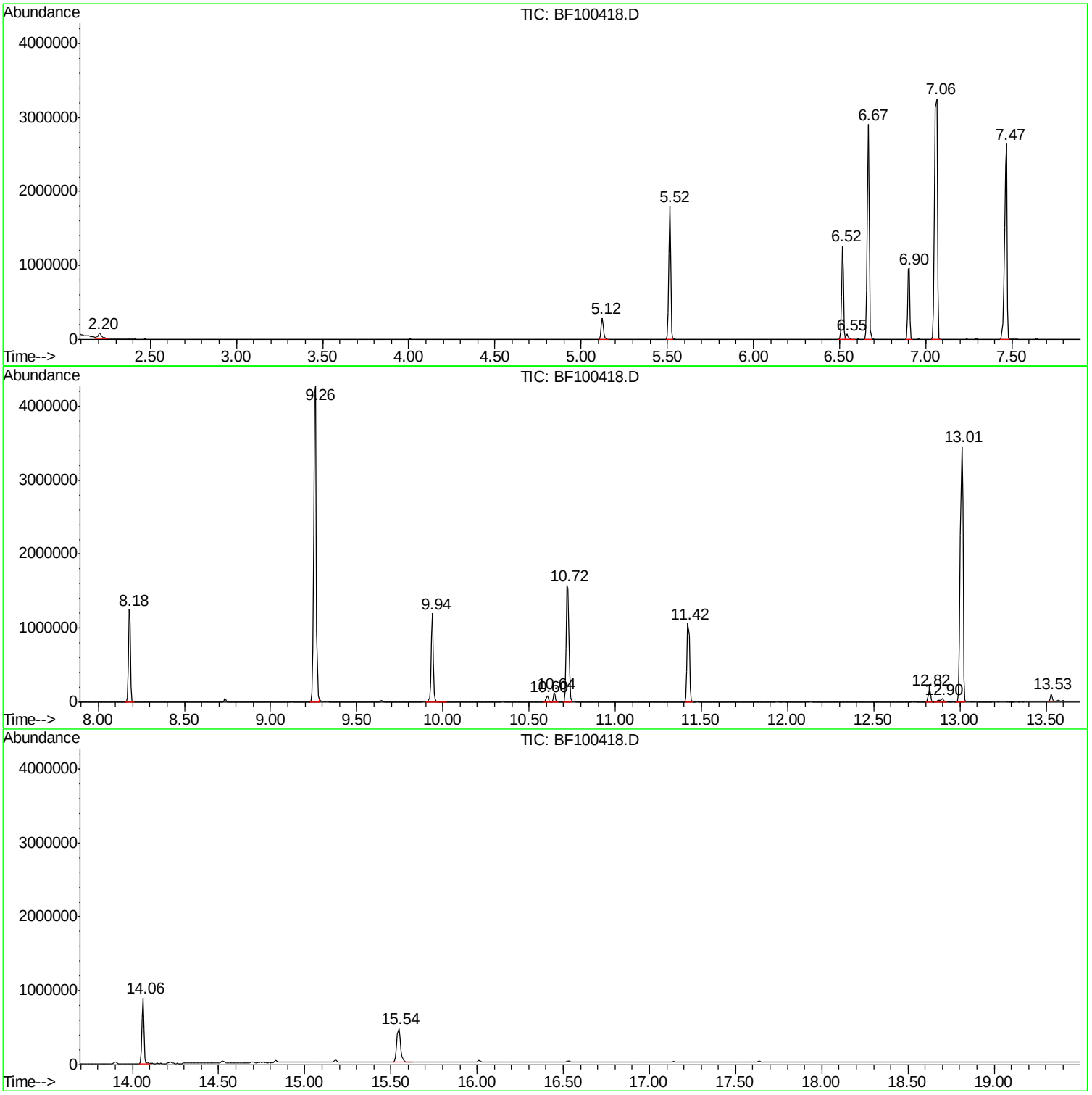
Sample : I6355-08
Misc :
ALS Vial : 36 Sample Multiplier: 1

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

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

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100418.D
Acq On : 11 Nov 2017 3:55
Operator : SJ/JU
Sample : I6355-08
Misc :
ALS Vial : 36 Sample Multiplier: 1

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

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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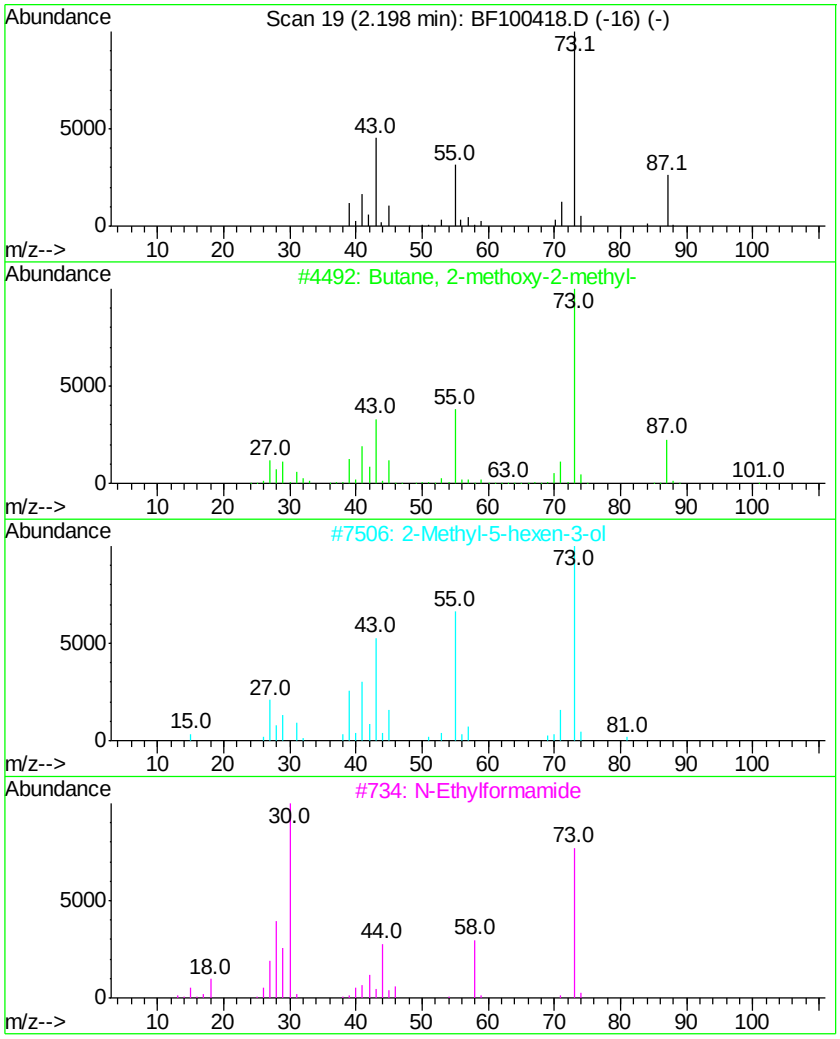
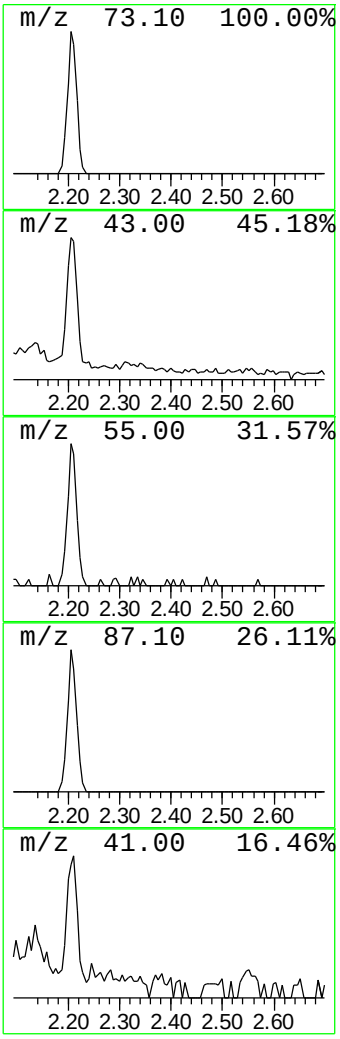
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.27 ng	100389	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	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





Library Search Compound Report

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Misc :
ALS Vial : 36 Sample Multiplier: 1

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

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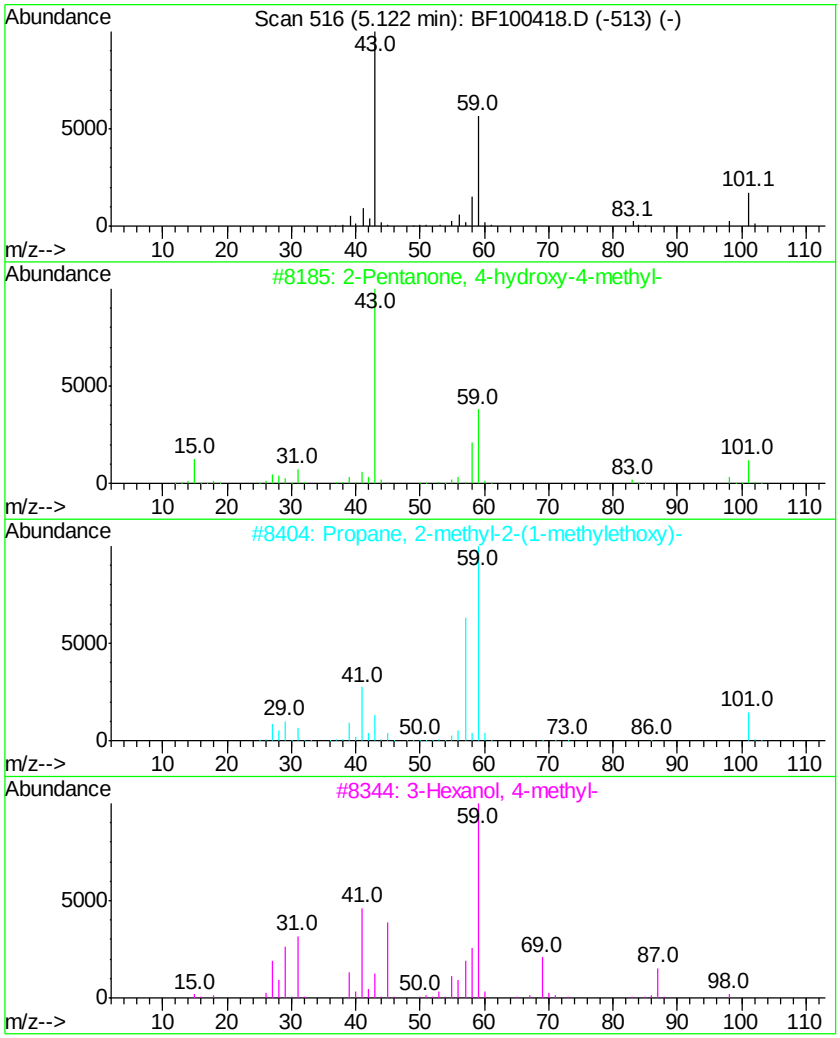
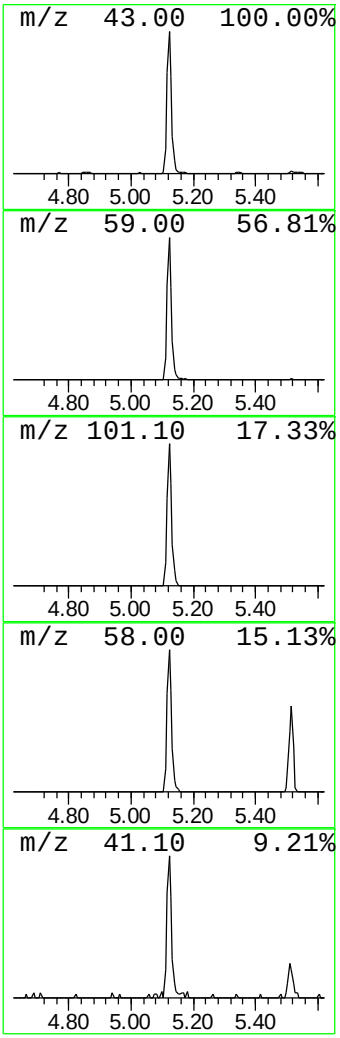
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.69 ng	295205	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	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Library Search Compound Report

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Data File : BF100418.D
Acq On : 11 Nov 2017 3:55
Operator : SJ/JU
Sample : I6355-08
Misc :
ALS Vial : 36 Sample Multiplier: 1

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

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
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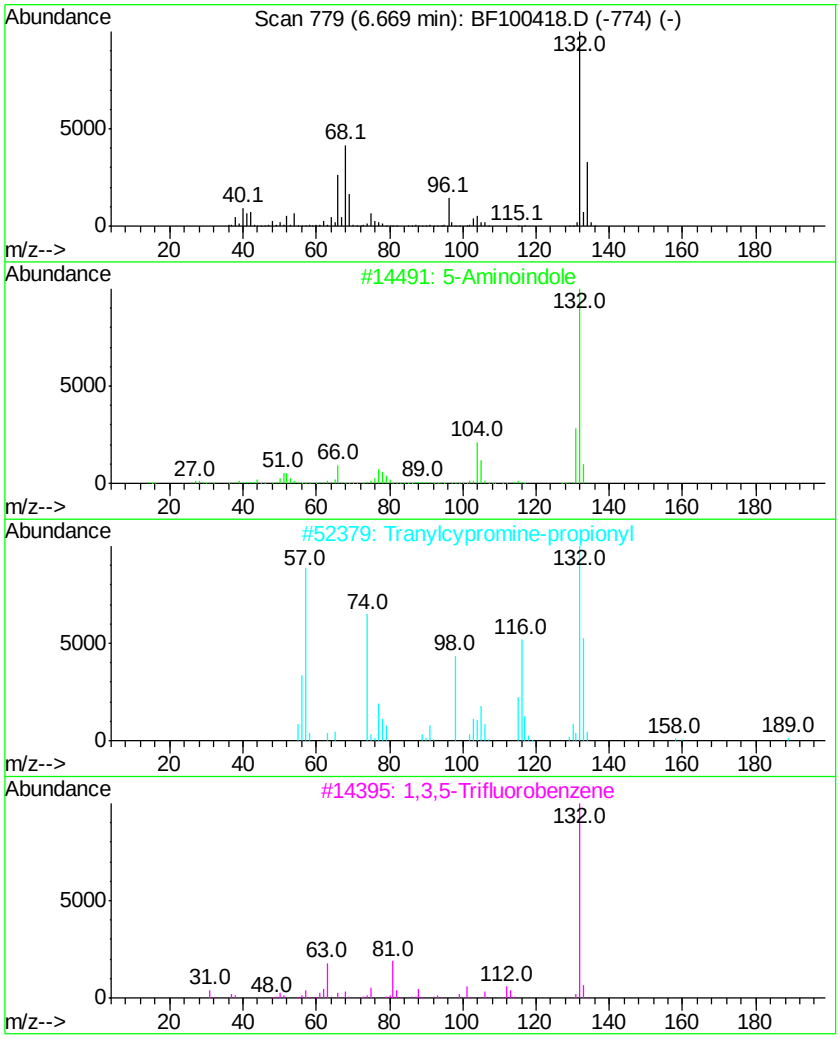
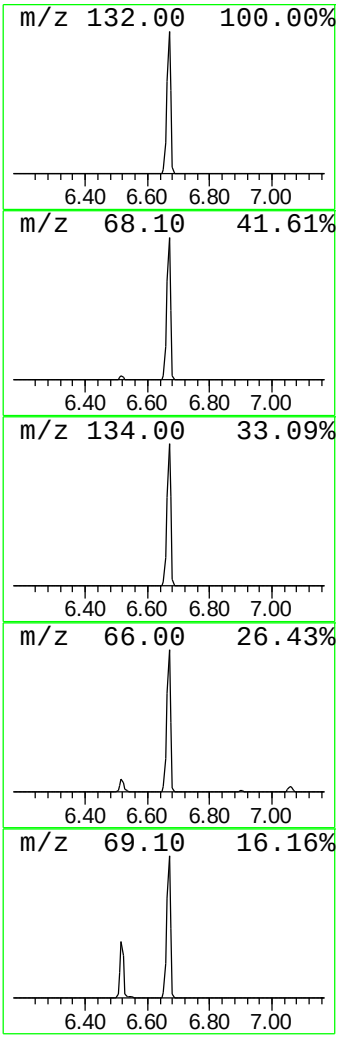
Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	58.44 ng	2579510	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : SJ/JU
Sample : I6355-08
Misc :
ALS Vial : 36 Sample Multiplier: 1

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

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

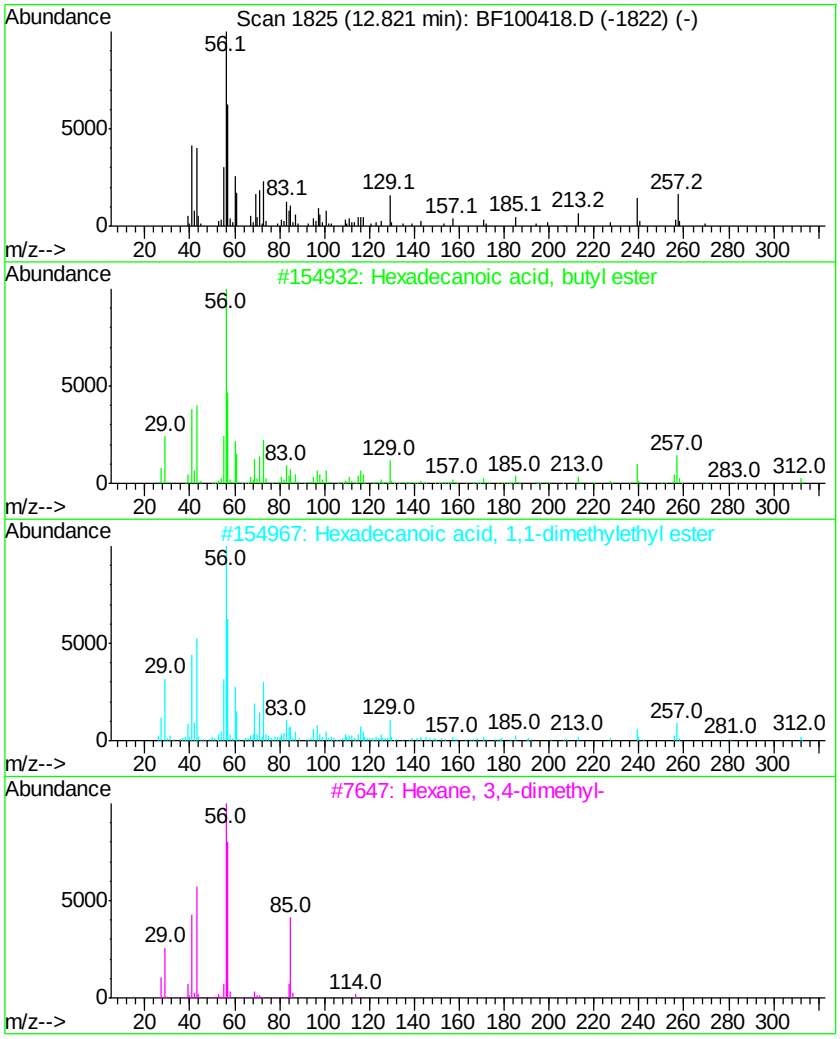
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

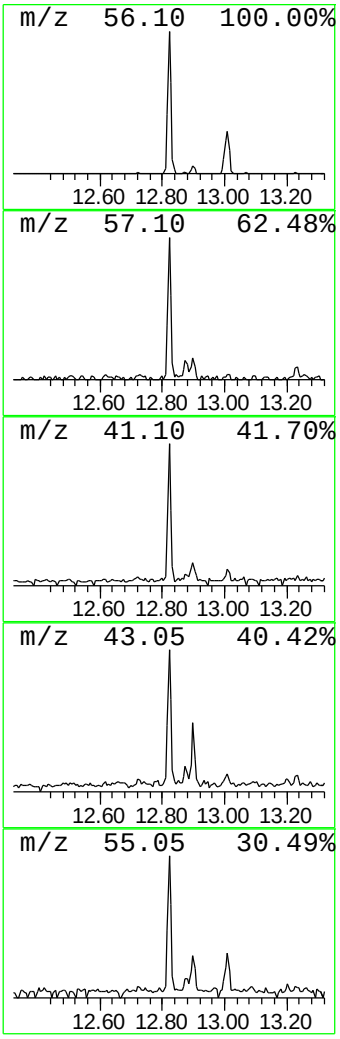
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	3.29 ng	130141	Chrysene-d12	14.06

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	91
3	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100418.D
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Operator : SJ/JU
Sample : I6355-08
Misc :
ALS Vial : 36 Sample Multiplier: 1

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

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

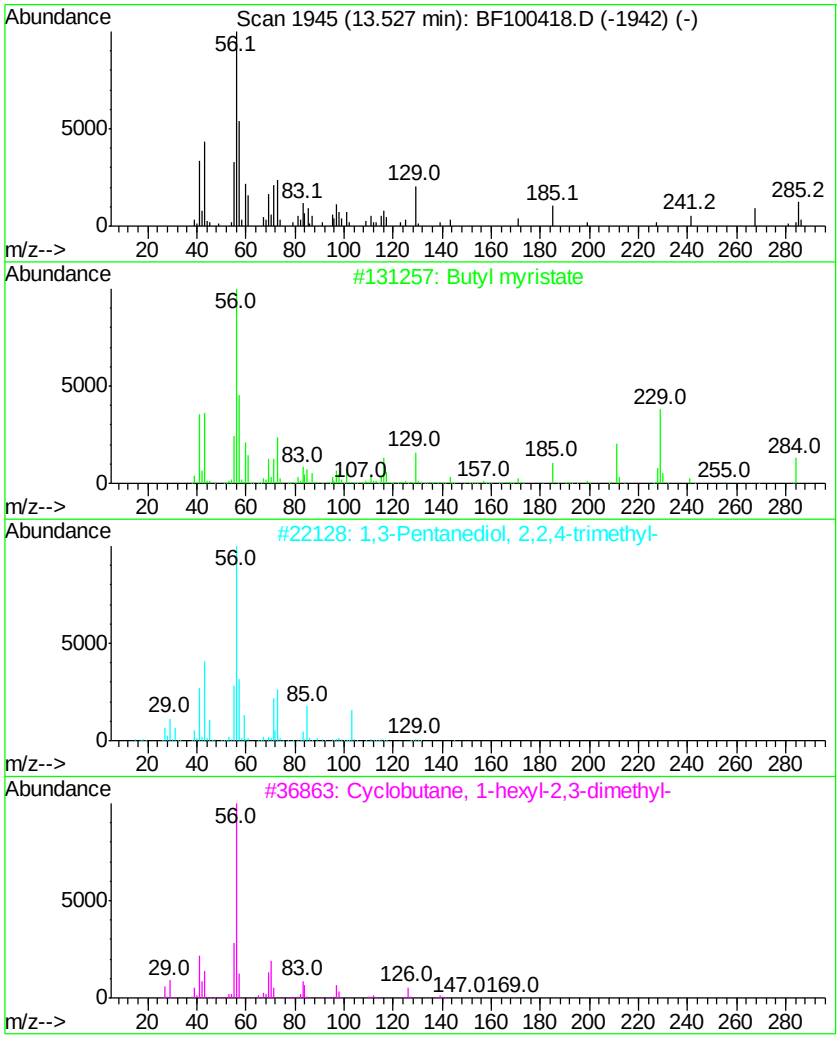
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

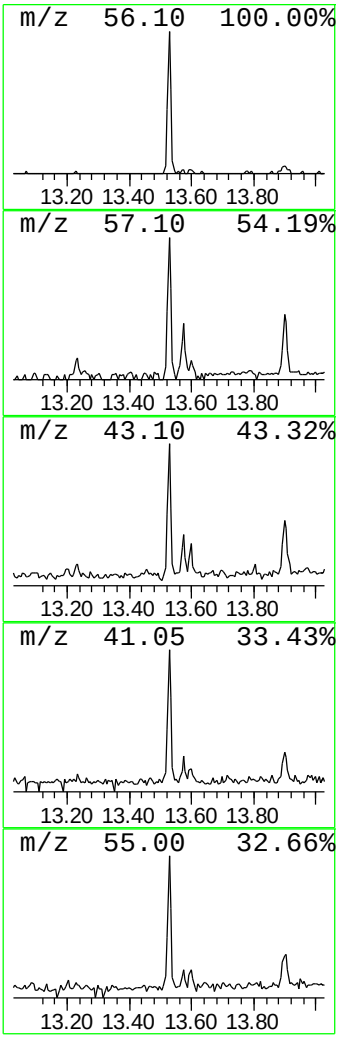
****

Peak Number 6 Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.18 ng	86160	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	72
2	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	38
3	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF111017\
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	2.3	ng	100389	1	6.90	882829	20.0
2-Pentanone, 4-hy...	5.12	6.7	ng	295205	1	6.90	882829	20.0
unknown6.67	6.67	58.4	ng	2579510	1	6.90	882829	20.0
Hexadecanoic acid...	12.82	3.3	ng	130141	5	14.06	791350	20.0
Butyl myristate	13.53	2.2	ng	86160	5	14.06	791350	20.0