LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
Data File : BF100495.D
Acq On : 12 Nov 2017 17:40
Operator : SJ/JU
Sample : I6403-08
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110817-TIDO-F-U-S

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	27	rVB	85820	119881	3.14%	0.531%
2	5.122	512	516	527	rBV	246785	264012	6.92%	1.169%
3	5.516	578	583	586	rBV	1404366	1264345	33.13%	5.597%
4	6.516	749	753	756	rBV	958705	822731	21.56%	3.642%
5	6.669	774	779	782	rBV	2335163	2137623	56.02%	9.463%
6	6.898	815	818	822	rVB	967150	813172	21.31%	3.600%
7	7.057	841	845	849	rBV	3010319	2837416	74.36%	12.560%
8	7.463	908	914	917	rBV	2287220	2344626	61.44%	10.379%
9	8.181	1032	1036	1040	rBV	1229891	999922	26.20%	4.426%
10	9.257	1214	1219	1222	rBV	3813474	3816038	100.00%	16.892%
11	9.645	1282	1285	1290	rBV	73810	61213	1.60%	0.271%
12	9.886	1323	1326	1329	rBV	143360	116572	3.05%	0.516%
13	9.939	1329	1335	1346	rVB	1006310	1000785	26.23%	4.430%
14	10.722	1464	1468	1478	rBV	1314260	1222705	32.04%	5.413%
15	11.422	1584	1587	1591	rBV	938967	771232	20.21%	3.414%
16	12.821	1822	1825	1828	rBV	122173	93922	2.46%	0.416%
17	13.010	1852	1857	1860	rBV	2828939	2599125	68.11%	11.506%
18	13.527	1941	1945	1948	rVB	80164	59957	1.57%	0.265%
19	14.063	2032	2036	2044	rVB	779488	724992	19.00%	3.209%
20	15.545	2282	2288	2297	rBV	358468	519971	13.63%	2.302%

Sum of corrected areas: 22590240

LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
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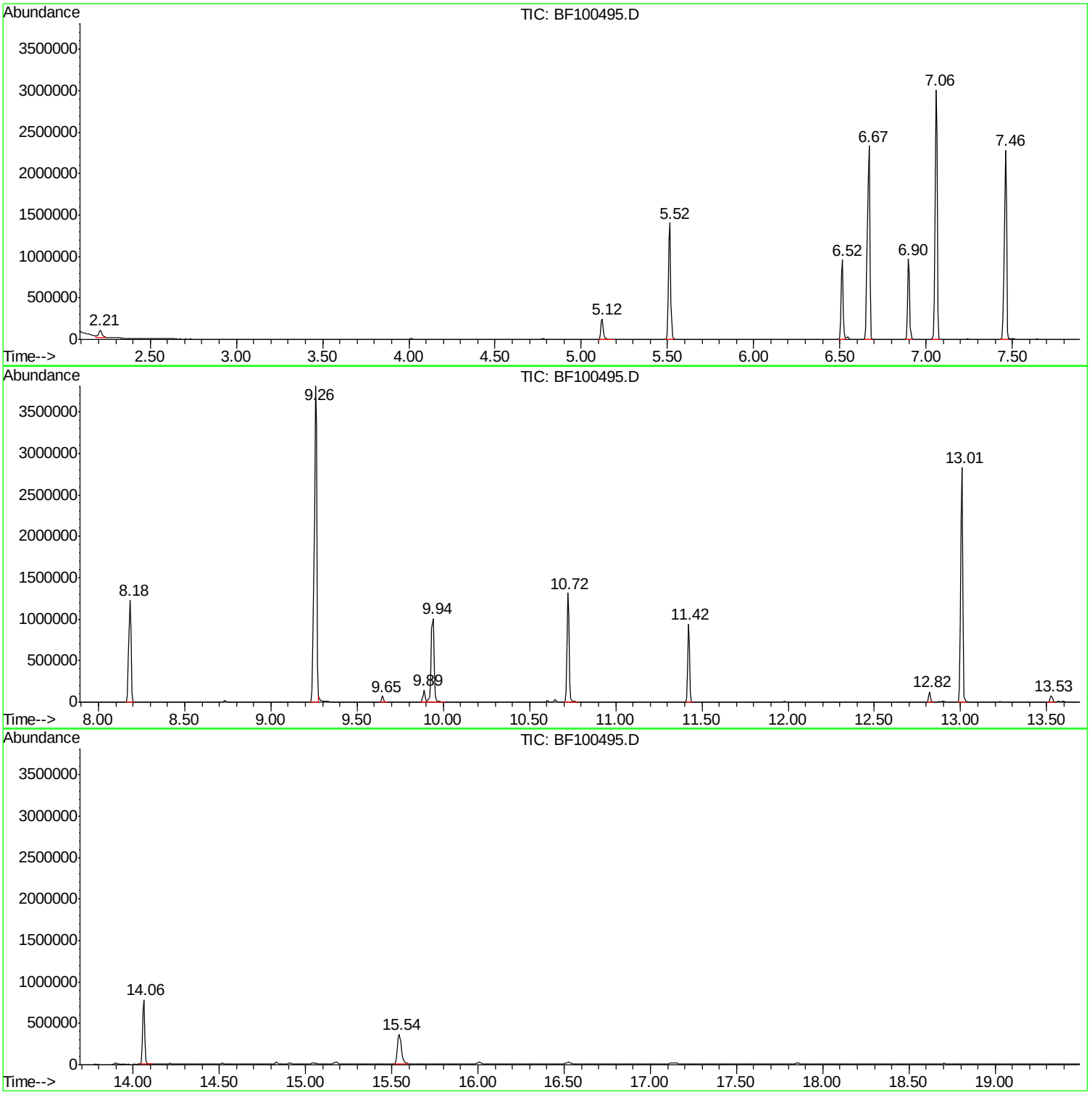
Acq On : 12 Nov 2017 17:40
Operator : SJ/JU
Sample : I6403-08
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110817-TIDO-F-U-S

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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Data File : BF100495.D
Acq On : 12 Nov 2017 17:40
Operator : SJ/JU
Sample : I6403-08
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110817-TIDO-F-U-S

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

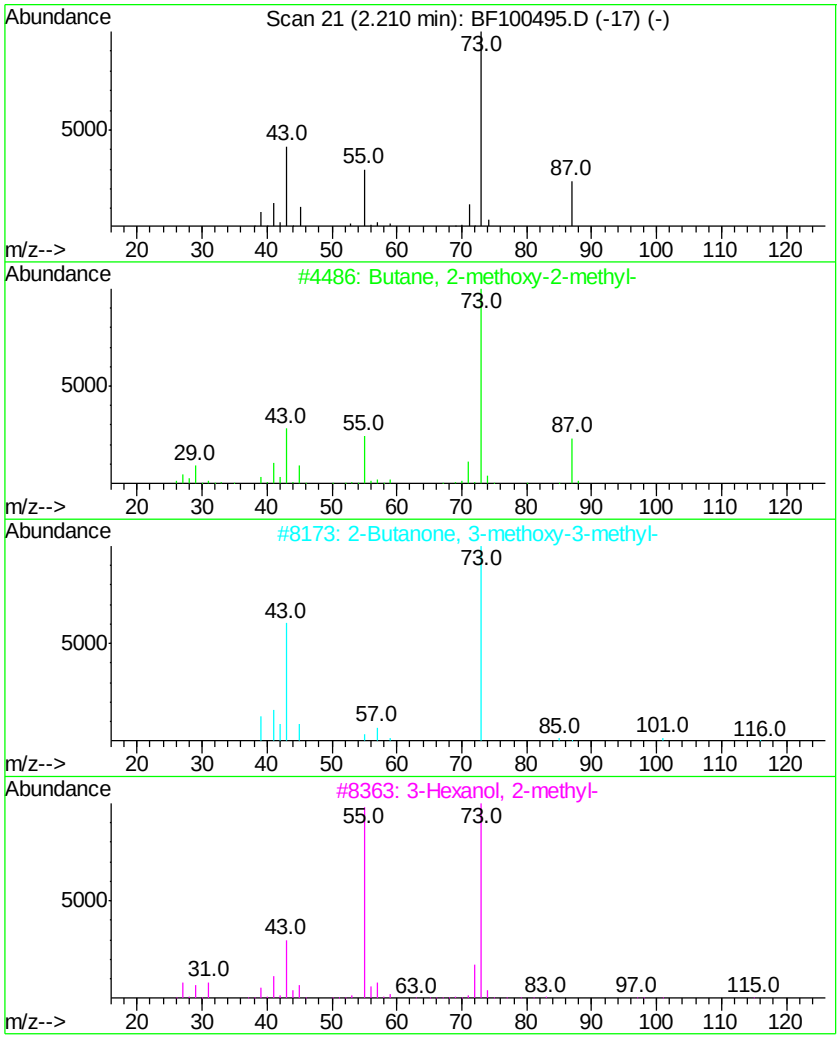
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

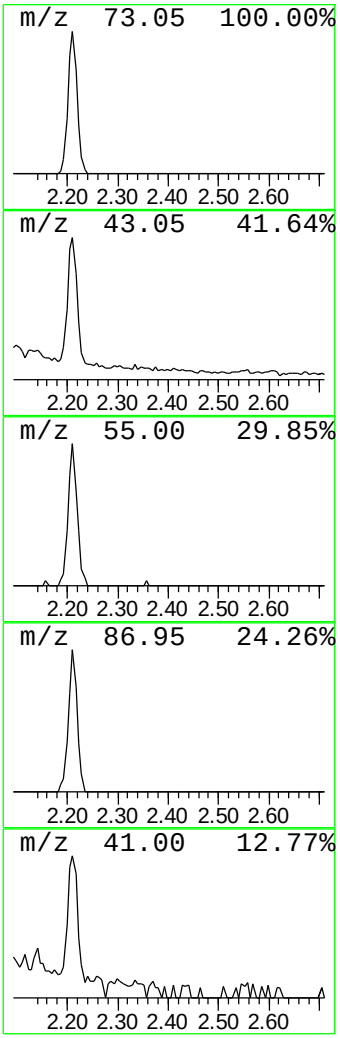
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	2.95 ng	119881	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	83
2	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	25
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
Data File : BF100495.D
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Operator : SJ/JU
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Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110817-TIDO-F-U-S

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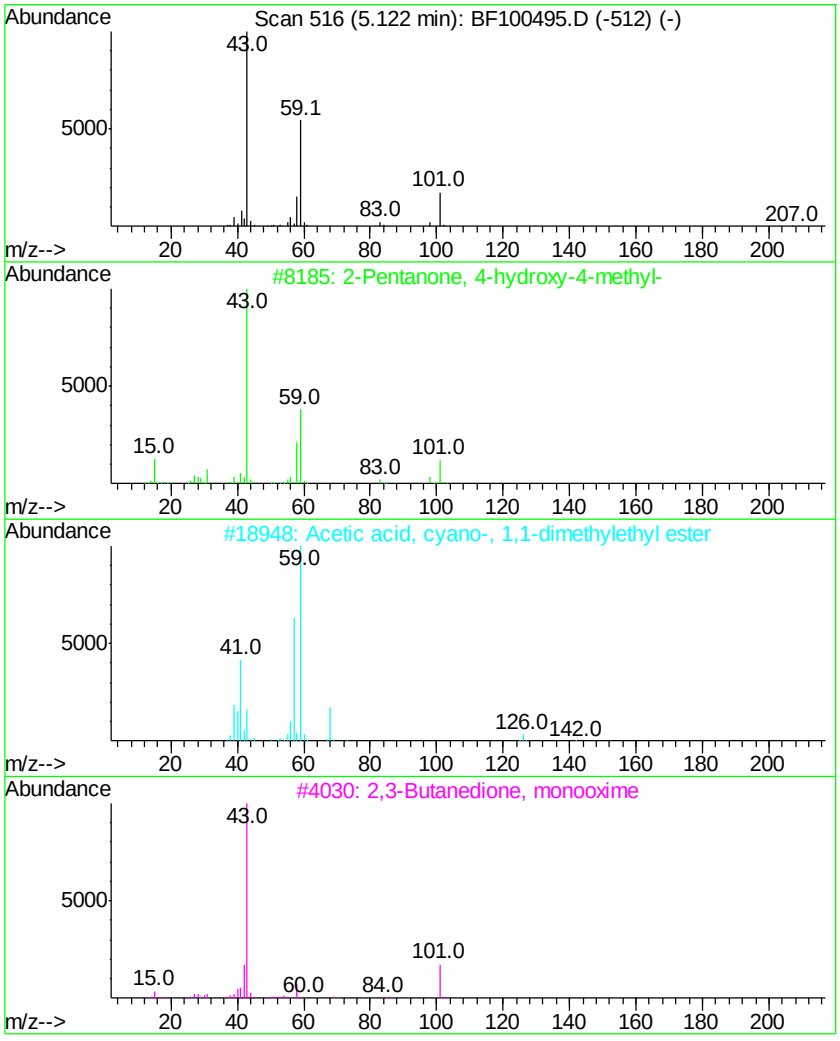
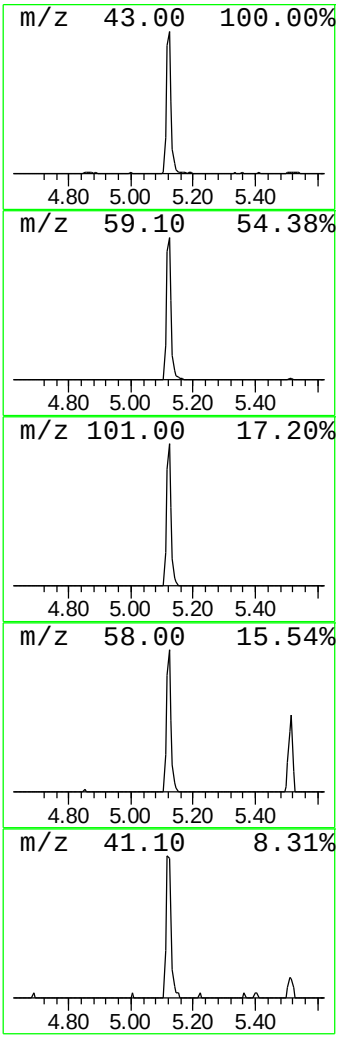
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.49 ng	264012	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

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Data File : BF100495.D
Acq On : 12 Nov 2017 17:40
Operator : SJ/JU
Sample : I6403-08
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110817-TIDO-F-U-S

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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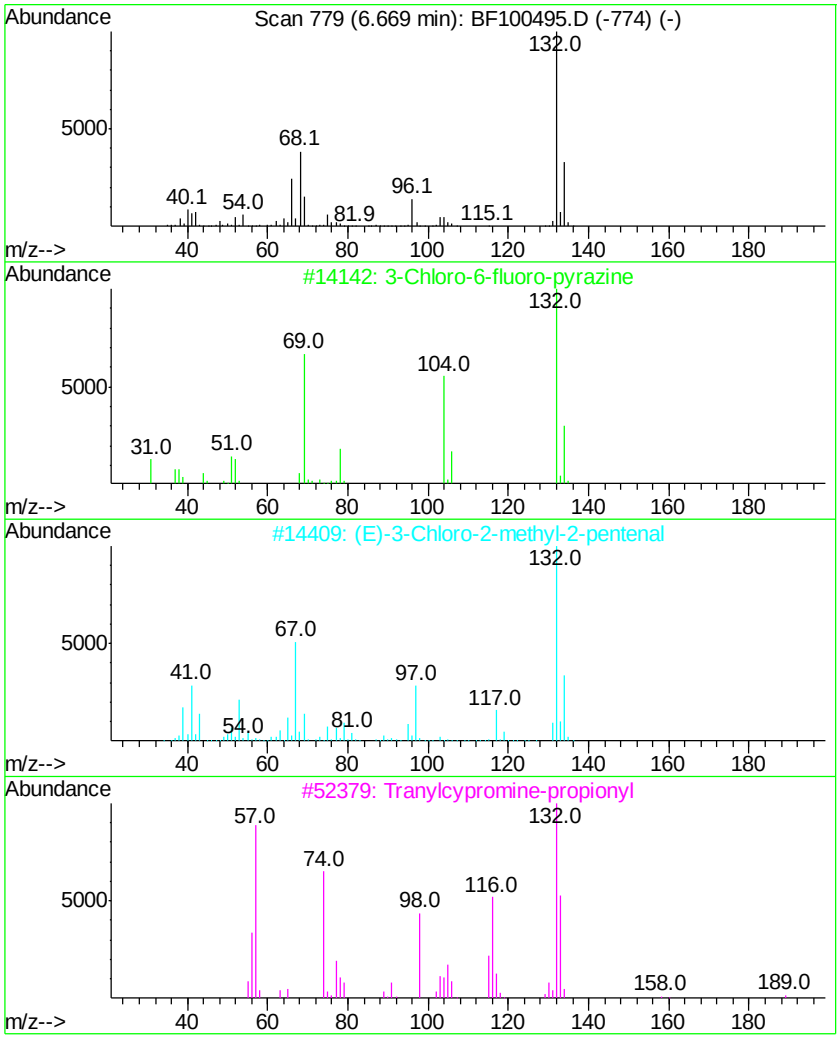
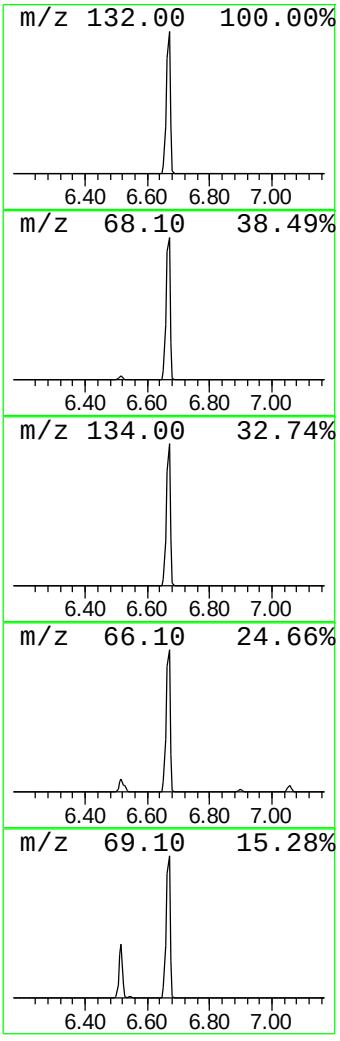
Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	52.57 ng	2137620	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Data File : BF100495.D
Acq On : 12 Nov 2017 17:40
Operator : SJ/JU
Sample : I6403-08
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110817-TIDO-F-U-S

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

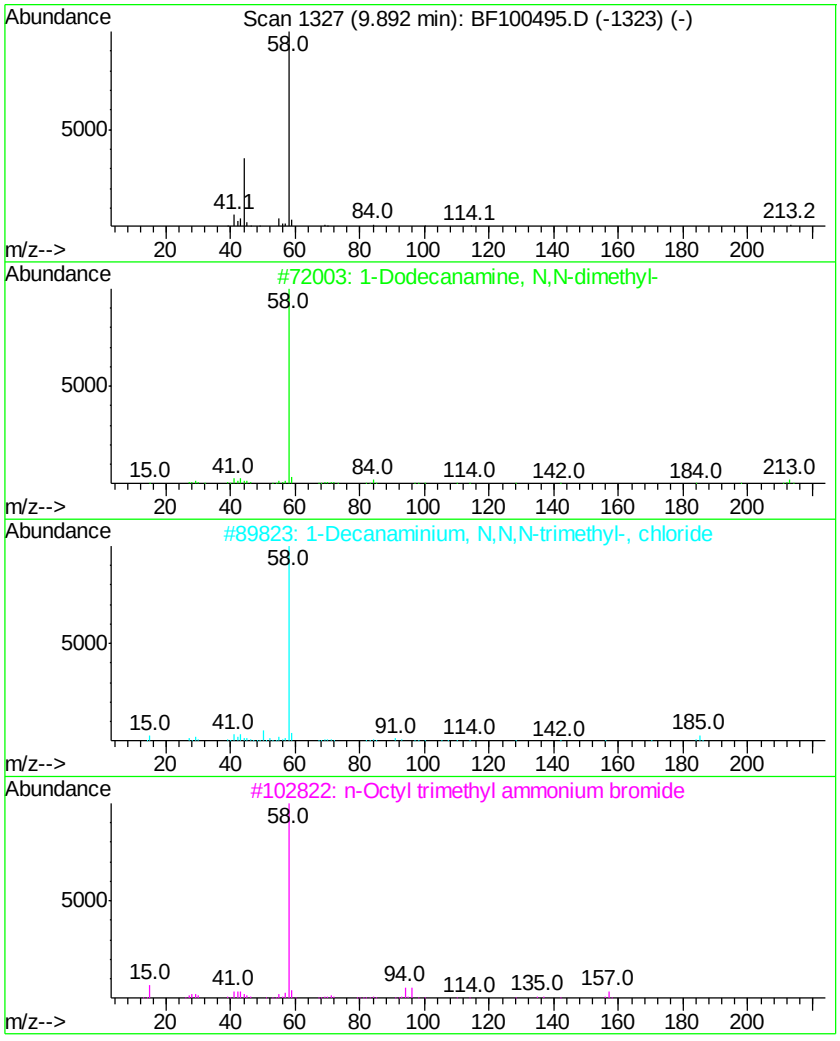
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

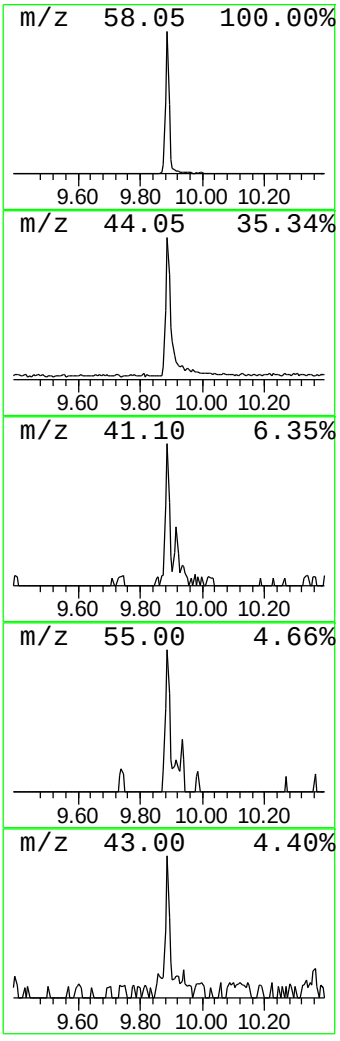
****

Peak Number 5 1-Dodecanamine, N,N-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.89	2.33 ng	116572	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	64
2	1-Decanaminium, N,N,N-trimethyl-...	235	C13H30ClN	010108-87-9	64
3	n-Octyl trimethyl ammonium bromide	251	C11H26BrN	002083-68-3	59
4	Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	59
5	1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	53





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111217\
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Operator : SJ/JU
Sample : I6403-08
Misc :
ALS Vial : 64 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110817-TIDO-F-U-S

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

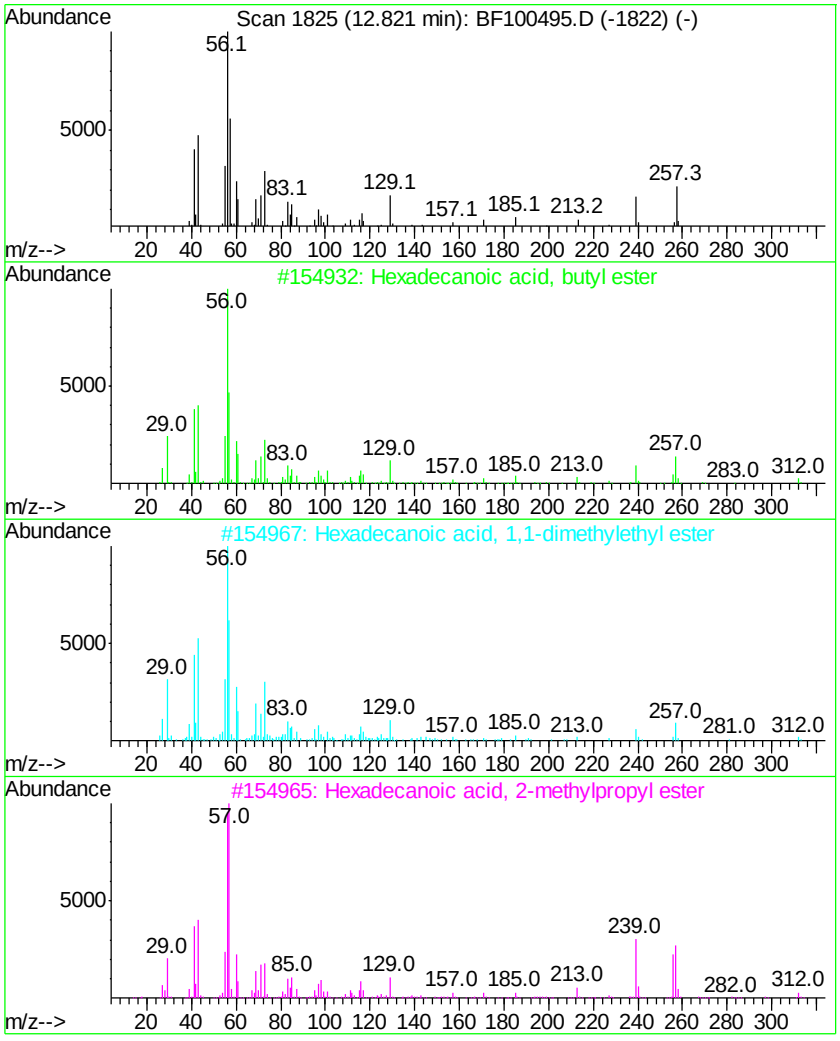
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

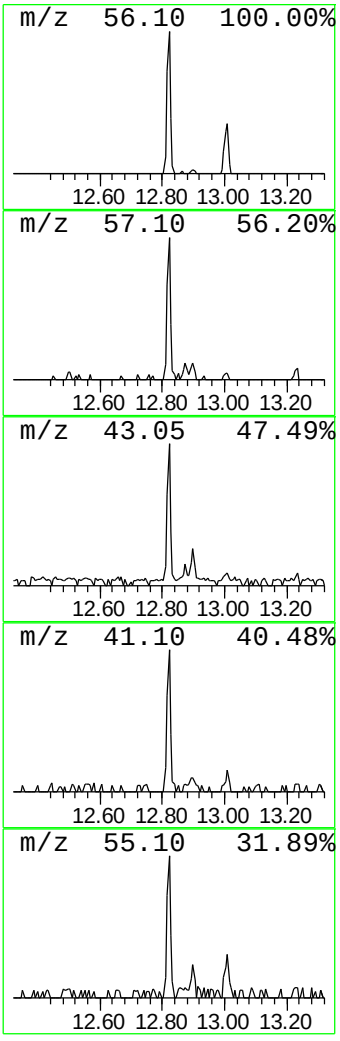
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.59 ng	93922	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	83
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	38
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.21	3.0	ng	119881	1	6.90	813172	20.0
2-Pentanone, 4-hy...	5.12	6.5	ng	264012	1	6.90	813172	20.0
unknown6.67	6.67	52.6	ng	2137620	1	6.90	813172	20.0
1-Dodecanamine, N...	9.89	2.3	ng	116572	3	9.94	1000790	20.0
Hexadecanoic acid...	12.82	2.6	ng	93922	5	14.06	724992	20.0