LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100462.D
Acq On : 12 Nov 2017 2:11
Operator : SJ/JU
Sample : I6369-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110617-JETT-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	2.204	16	20	26	rVB	67362	87020	2.42%	0.383%
2	5.122	512	516	523	rBV	245646	248830	6.93%	1.095%
3	5.516	579	583	586	rBV	1453223	1249780	34.80%	5.499%
4	6.516	749	753	757	rBV	991267	836320	23.29%	3.680%
5	6.669	775	779	782	rBV	2395077	2087565	58.13%	9.185%
6	6.904	815	819	822	rBV	1018414	867198	24.15%	3.816%
7	7.063	841	846	849	rBV	2806091	2753828	76.68%	12.117%
8	7.463	909	914	917	rBV	2093401	2241650	62.42%	9.863%
9	8.180	1033	1036	1040	rBV	1139993	1037909	28.90%	4.567%
10	8.733	1127	1130	1134	rBV	110320	93438	2.60%	0.411%
11	9.257	1214	1219	1223	rBV	3593957	3591106	100.00%	15.801%
12	9.645	1282	1285	1289	rBV	98757	81361	2.27%	0.358%
13	9.939	1329	1335	1348	rVB	1071220	1000843	27.87%	4.404%
14	10.604	1445	1448	1452	rVB	99089	71813	2.00%	0.316%
15	10.651	1452	1456	1459	rBV	276733	241904	6.74%	1.064%
16	10.727	1464	1469	1478	rBV	1148450	1130320	31.48%	4.973%
17	11.427	1584	1588	1591	rBV	851599	771996	21.50%	3.397%
18	13.010	1853	1857	1860	rBV	2840339	2587814	72.06%	11.387%
19	13.898	2005	2008	2015	rVB5	24362	37269	1.04%	0.164%
20	14.062	2032	2036	2043	rBV	928278	834858	23.25%	3.673%
21	15.398	2261	2263	2269	rBV7	28024	38191	1.06%	0.168%
22	15.545	2284	2288	2295	rVB	399251	570266	15.88%	2.509%
23	15.698	2311	2314	2319	rVB6	41192	50227	1.40%	0.221%
24	16.274	2407	2412	2419	rVB5	54914	111871	3.12%	0.492%
25	16.715	2482	2487	2493	rVB2	58481	103586	2.88%	0.456%

Sum of corrected areas: 22726963

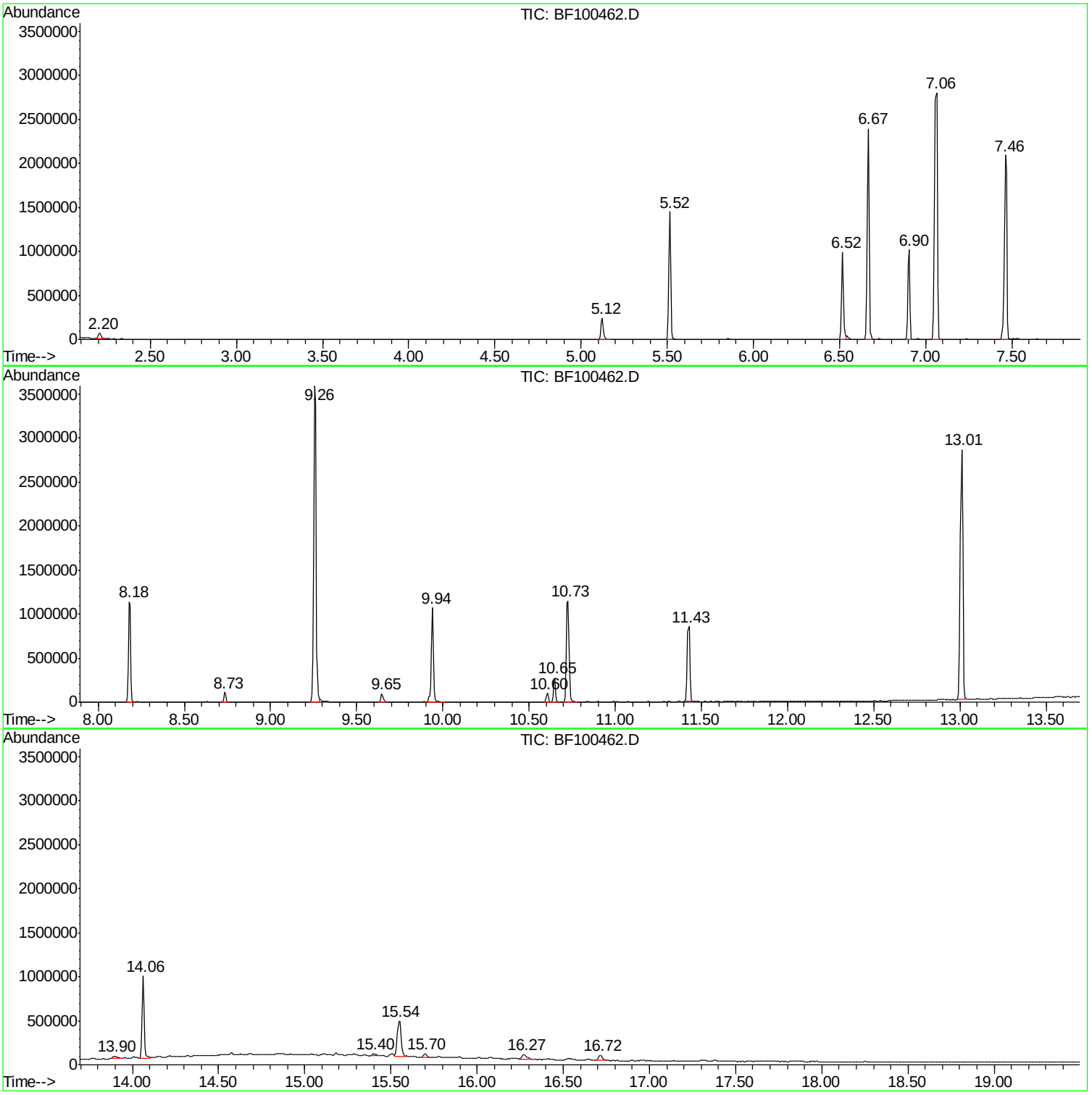
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
Data File : BF100462.D
Acq On : 12 Nov 2017 2:11
Operator : SJ/JU
Sample : I6369-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110617-JETT-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



Library Search Compound Report

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Data File : BF100462.D
Acq On : 12 Nov 2017 2:11
Operator : SJ/JU
Sample : I6369-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110617-JETT-F-U-S

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

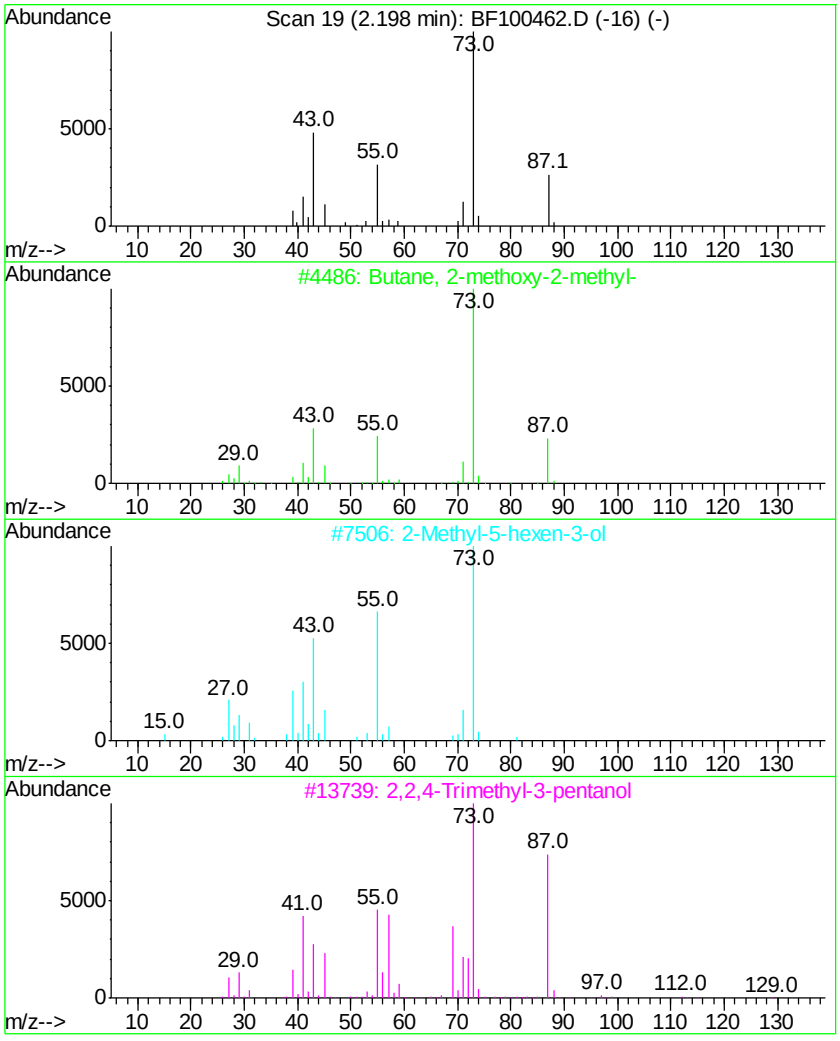
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

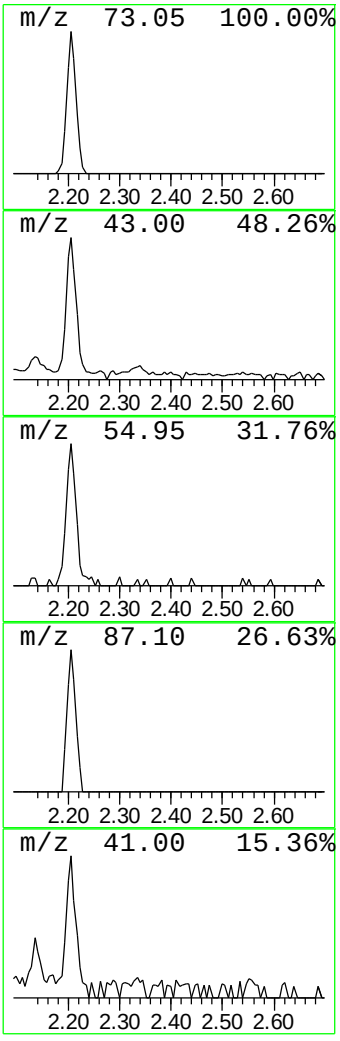
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.01 ng	87020	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-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	38
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF100462.D
Acq On : 12 Nov 2017 2:11
Operator : SJ/JU
Sample : I6369-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110617-JETT-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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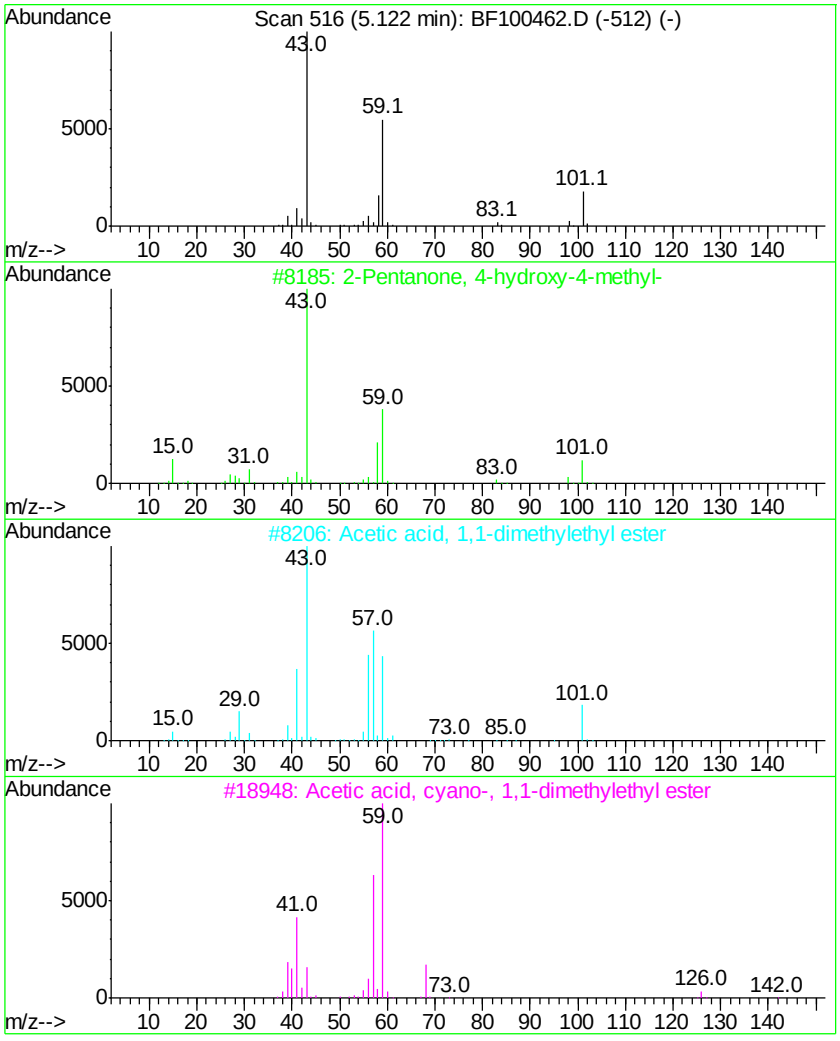
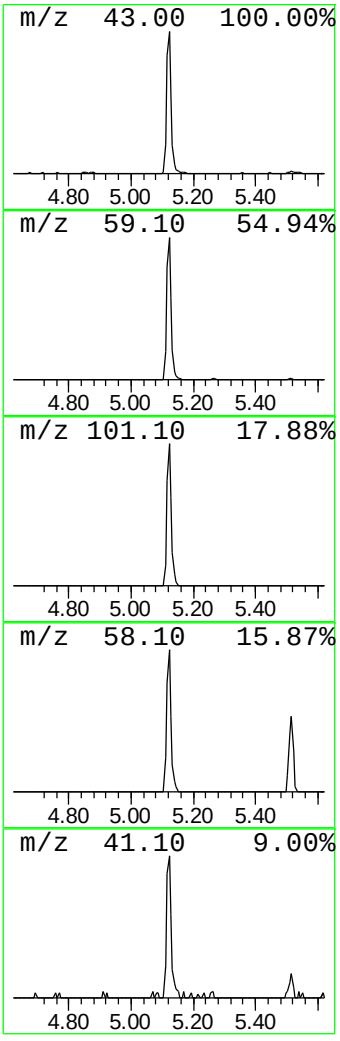
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	5.74 ng	248830	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

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Data File : BF100462.D
Acq On : 12 Nov 2017 2:11
Operator : SJ/JU
Sample : I6369-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110617-JETT-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
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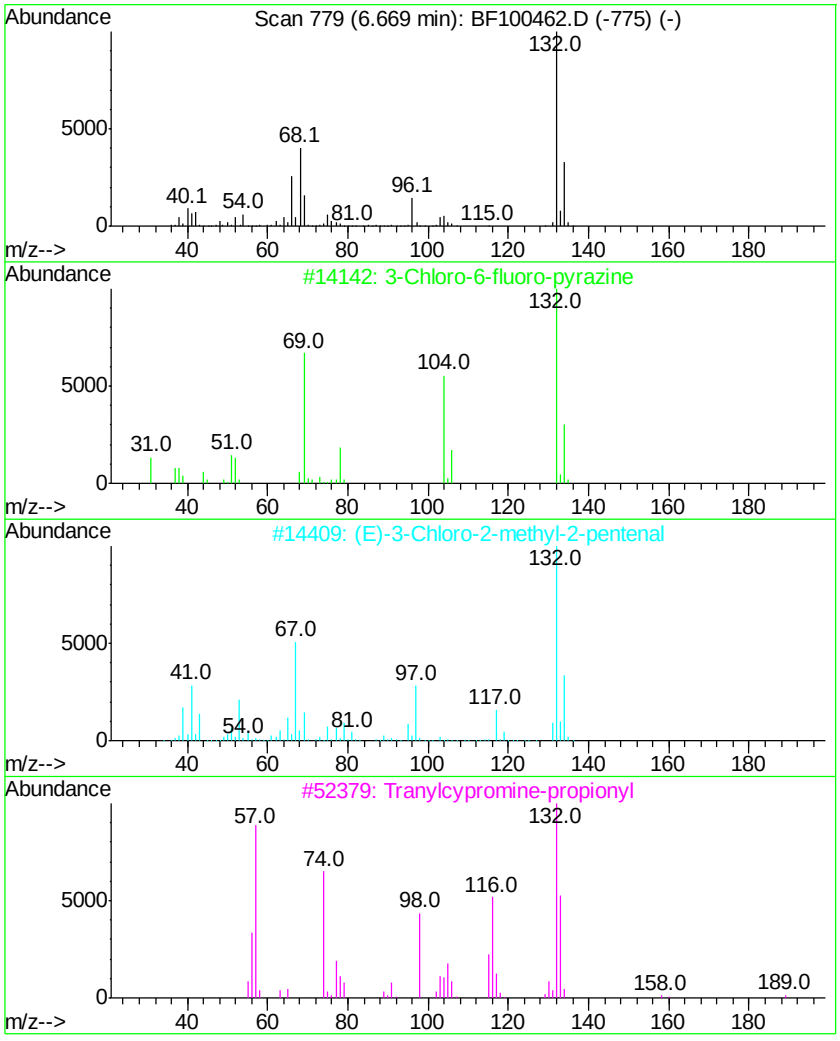
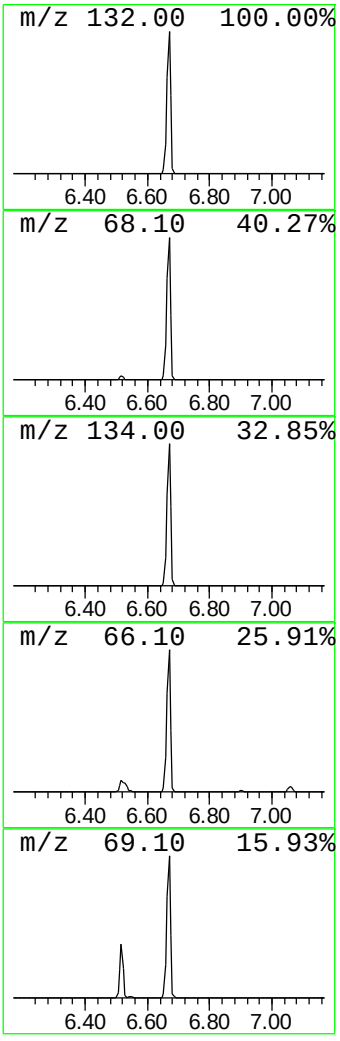
Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	48.15 ng	2087570	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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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





Library Search Compound Report

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Operator : SJ/JU
Sample : I6369-08
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110617-JETT-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
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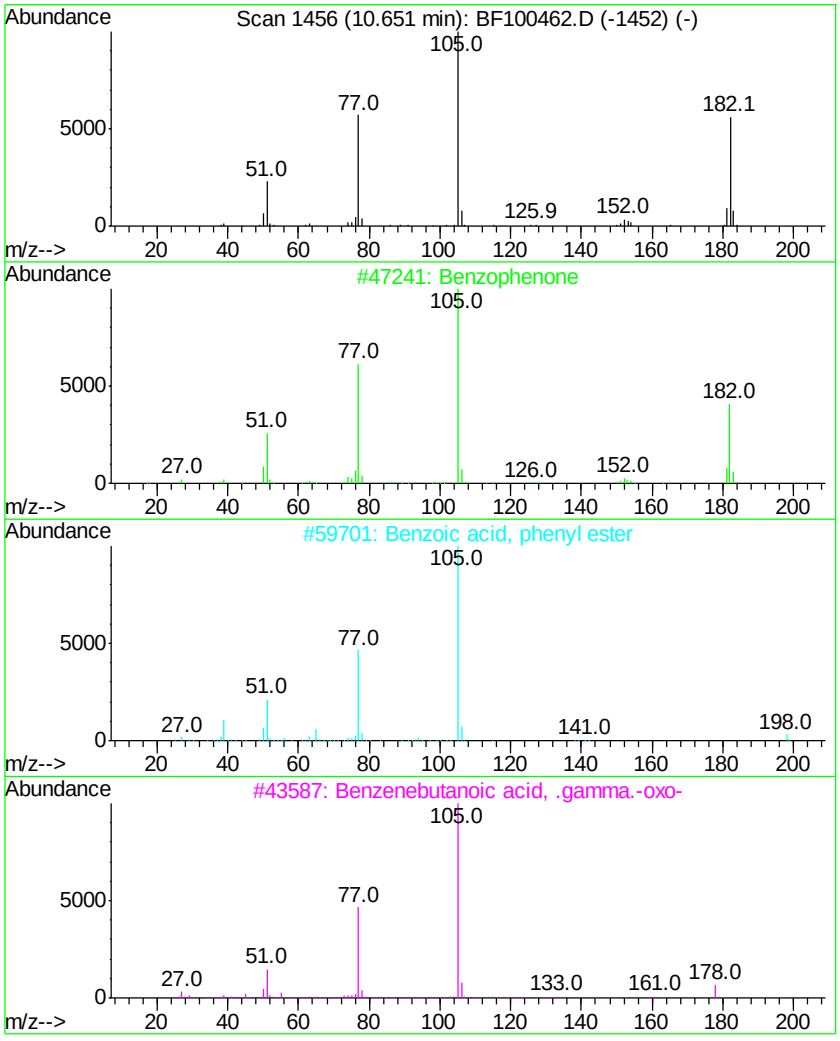
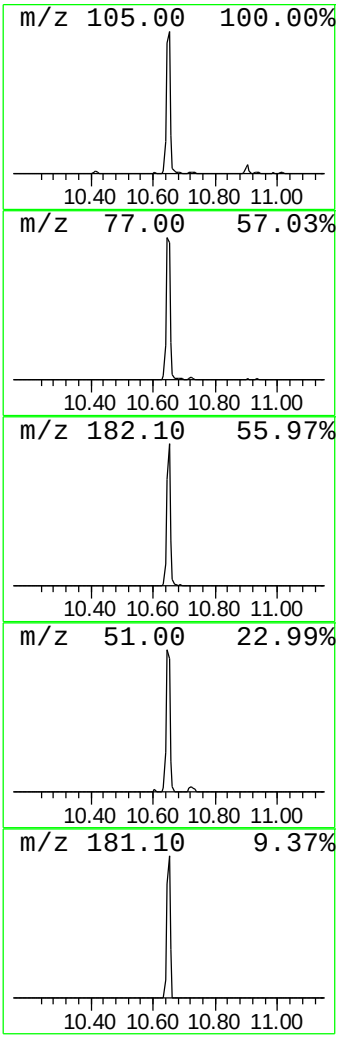
Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	4.83 ng	241904	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111117\
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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110617-JETT-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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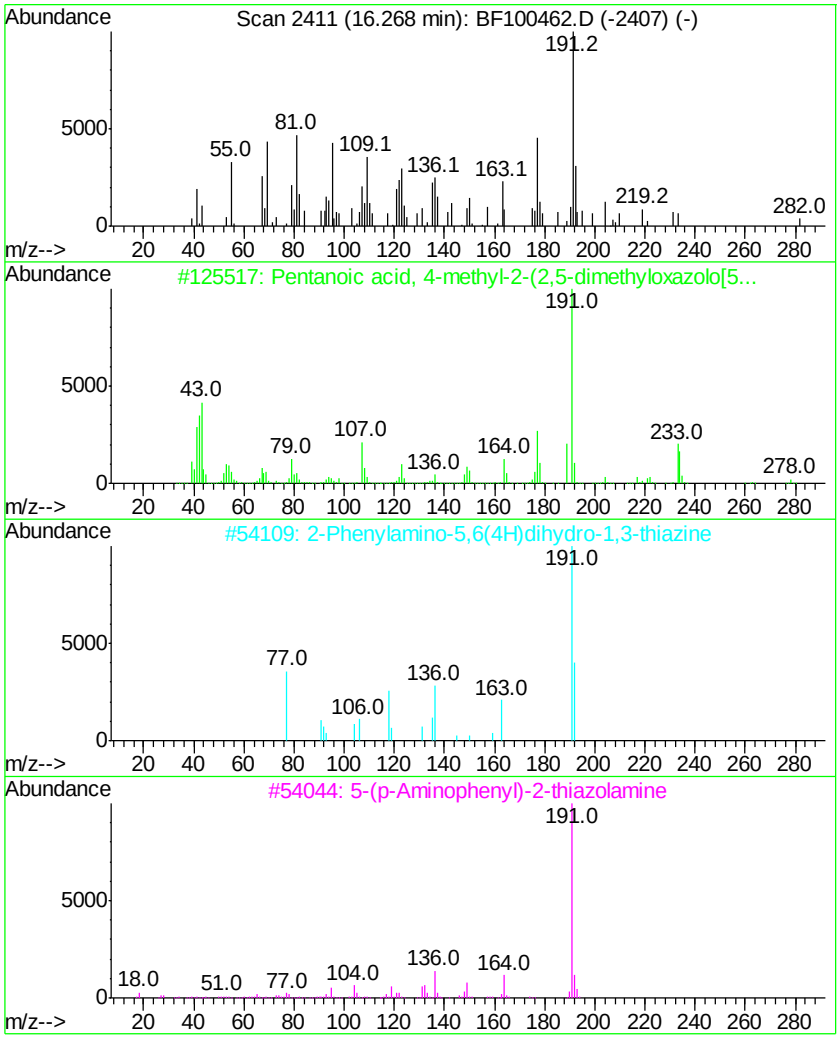
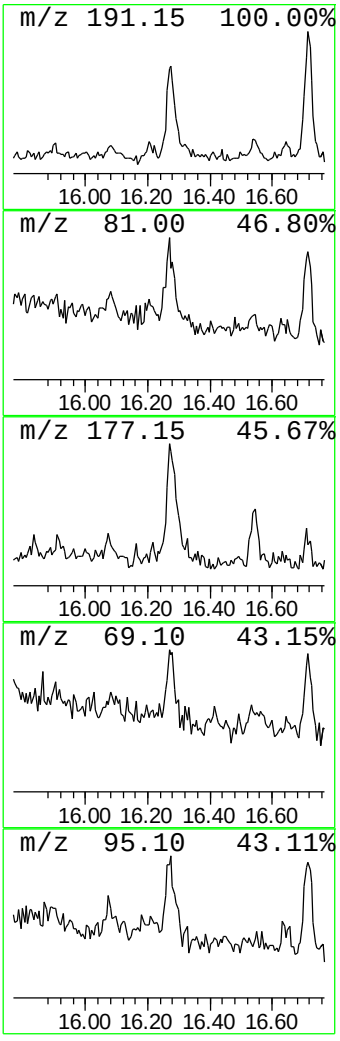
****

Peak Number 6 unknown16.27 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	3.92 ng	111871	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4-methyl-2-(2,5-...	278	C13H18N4O3	1000294-63-5	35
2	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	30
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	25
4	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	25
5	2-(2-Hydroxyethylimino)-3,6-dime...	222	C11H14N2OS	068720-70-7	22





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Instrument : BNA_F
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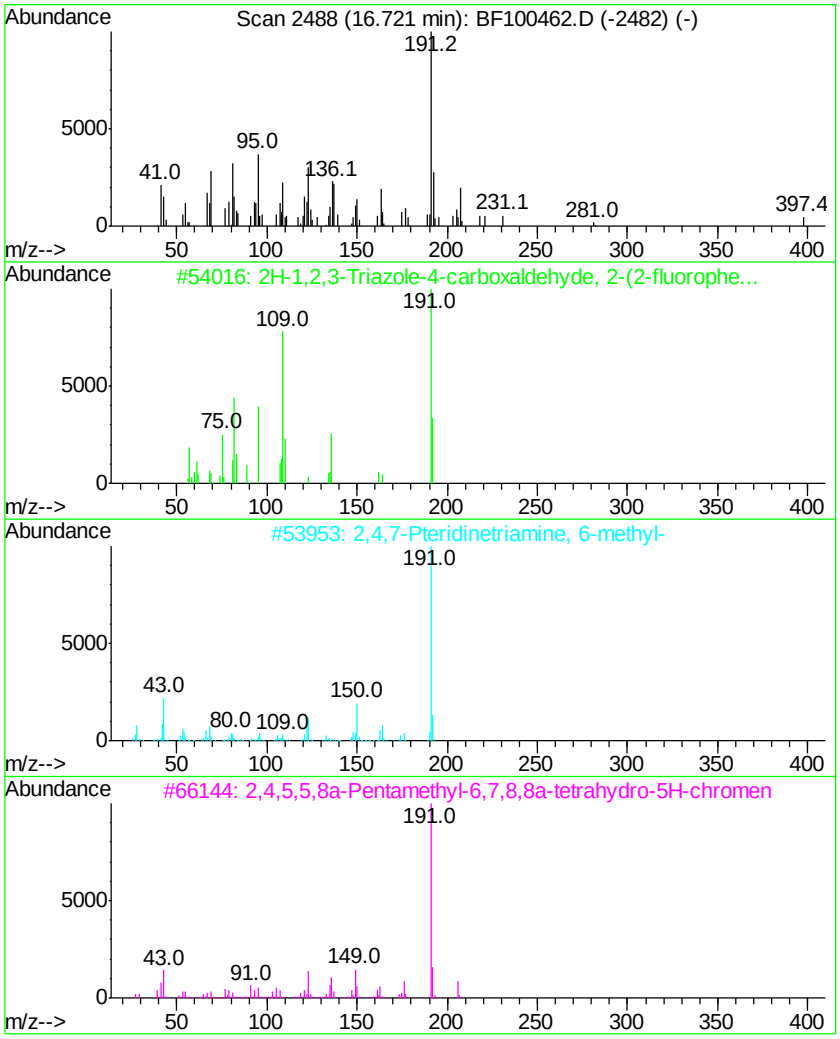
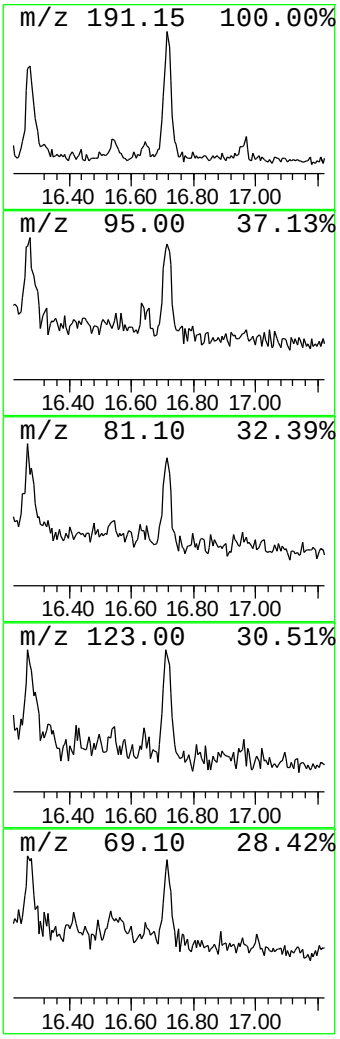
Peak Number 7 2H-1,2,3-Triazole-4-carboxa... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	3.63 ng	103586	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	50
2	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	43
3	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	43
4	9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	38
5	2,5,5,8a-Tetramethyl-4-methylene...	206	C14H22O	093175-76-9	38





Tentatively Identified Compound (LSC) summary

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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	2.0	ng	87020	1	6.90	867198	20.0
2-Pentanone, 4-hy...	5.12	5.7	ng	248830	1	6.90	867198	20.0
unknown6.67	6.67	48.1	ng	2087570	1	6.90	867198	20.0
Benzophenone	10.65	4.8	ng	241904	3	9.94	1000840	20.0
unknown16.27	16.27	3.9	ng	111871	6	15.55	570266	20.0
2H-1,2,3-Triazole...	16.72	3.6	ng	103586	6	15.55	570266	20.0