LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104514.D
Acq On : 14 Apr 2018 9:19
Operator : JU/SJ
Sample : J2368-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRI-E-D-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-BF040618.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	5.004	492	496	504	rVB	90747	93911	2.67%	0.473%
2	5.422	563	567	570	rBV	1145900	981667	27.90%	4.943%
3	6.439	736	740	745	rBV	687344	627454	17.84%	3.160%
4	6.575	759	763	767	rBV	1974967	1803303	51.26%	9.081%
5	6.804	799	802	806	rBV	766357	688122	19.56%	3.465%
6	6.963	825	829	833	rBV	2667204	2463738	70.03%	12.406%
7	7.375	893	899	902	rBV	1987839	1963387	55.81%	9.887%
8	8.092	1017	1021	1024	rBV	1083405	897962	25.53%	4.522%
9	9.169	1199	1204	1207	rBV	3727850	3517927	100.00%	17.715%
10	9.557	1267	1270	1279	rBV	111106	96571	2.75%	0.486%
11	9.845	1314	1319	1332	rVB	1027281	953135	27.09%	4.800%
12	10.274	1385	1392	1395	rBV2	39798	36560	1.04%	0.184%
13	10.639	1449	1454	1465	rVB	1193411	1162103	33.03%	5.852%
14	10.745	1470	1472	1477	rBV	39876	36712	1.04%	0.185%
15	11.333	1568	1572	1576	rBV	886840	743787	21.14%	3.745%
16	12.739	1808	1811	1814	rBV	125837	103284	2.94%	0.520%
17	12.927	1838	1843	1846	rBV	2558057	2447819	69.58%	12.326%
18	13.451	1928	1932	1935	rVB	69822	62216	1.77%	0.313%
19	13.821	1990	1995	2004	rBV	68592	79336	2.26%	0.400%
20	13.980	2018	2022	2027	rVB	676931	600877	17.08%	3.026%
21	15.445	2266	2271	2282	rBV	386733	498657	14.17%	2.511%

Sum of corrected areas: 19858528

LSC Report - Integrated Chromatogram

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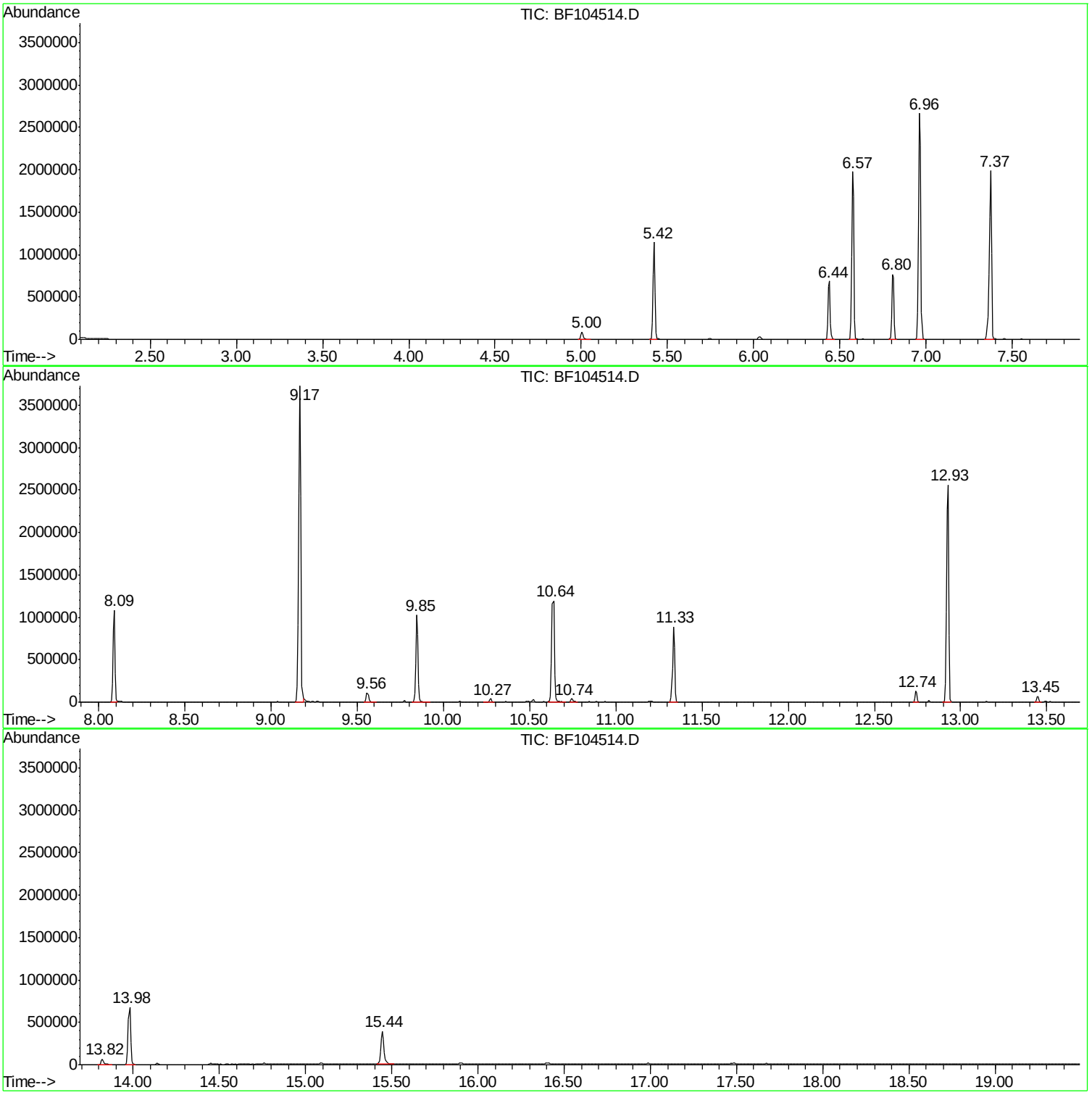
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRI-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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 : BF104514.D
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Sample : J2368-08
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Instrument : BNA_F
ClientSampleId : 041118-DBRI-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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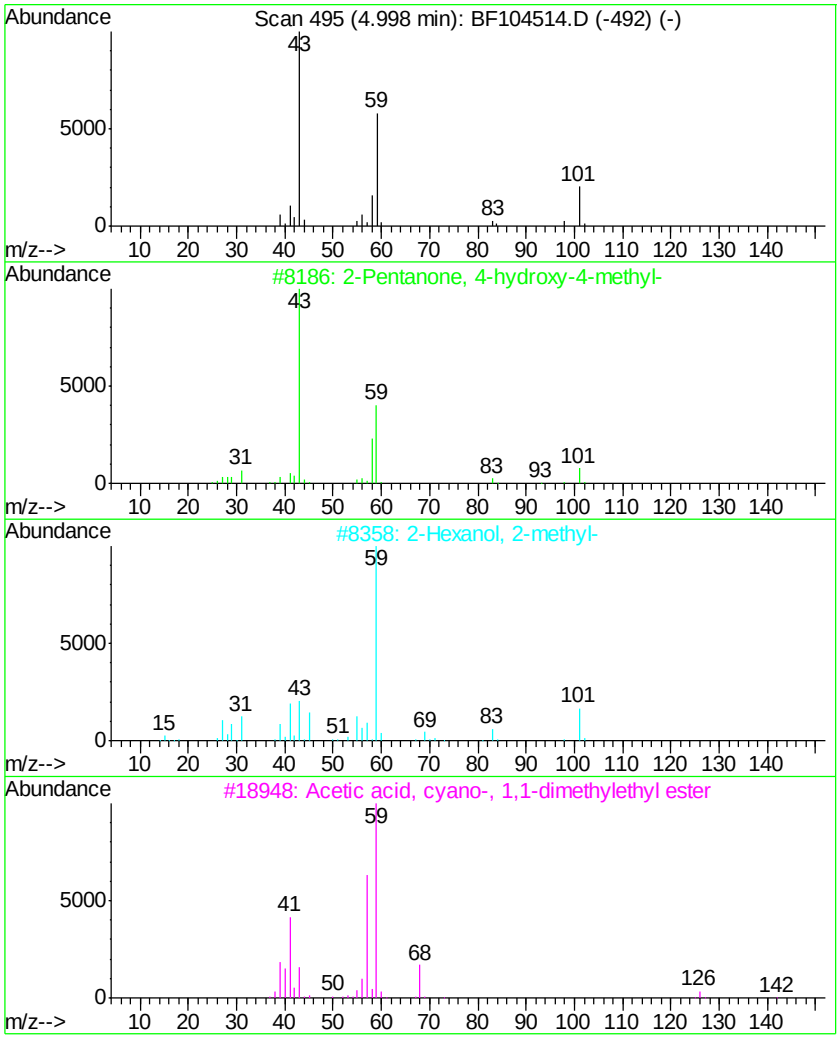
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

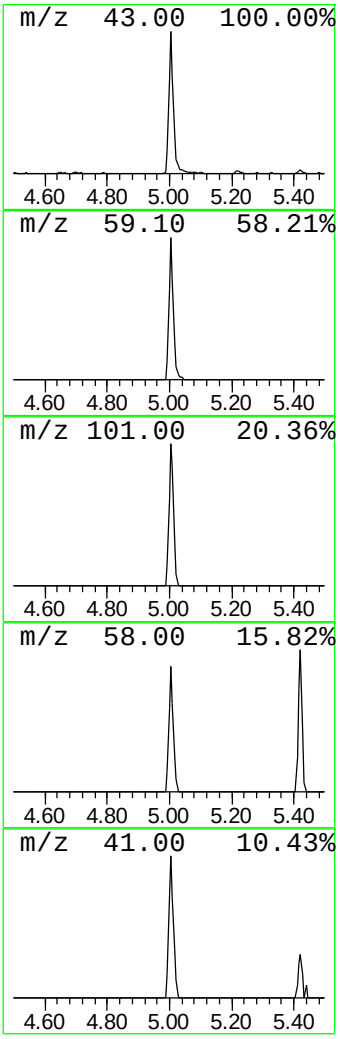
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.73 ng	93911	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : JU/SJ
Sample : J2368-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRI-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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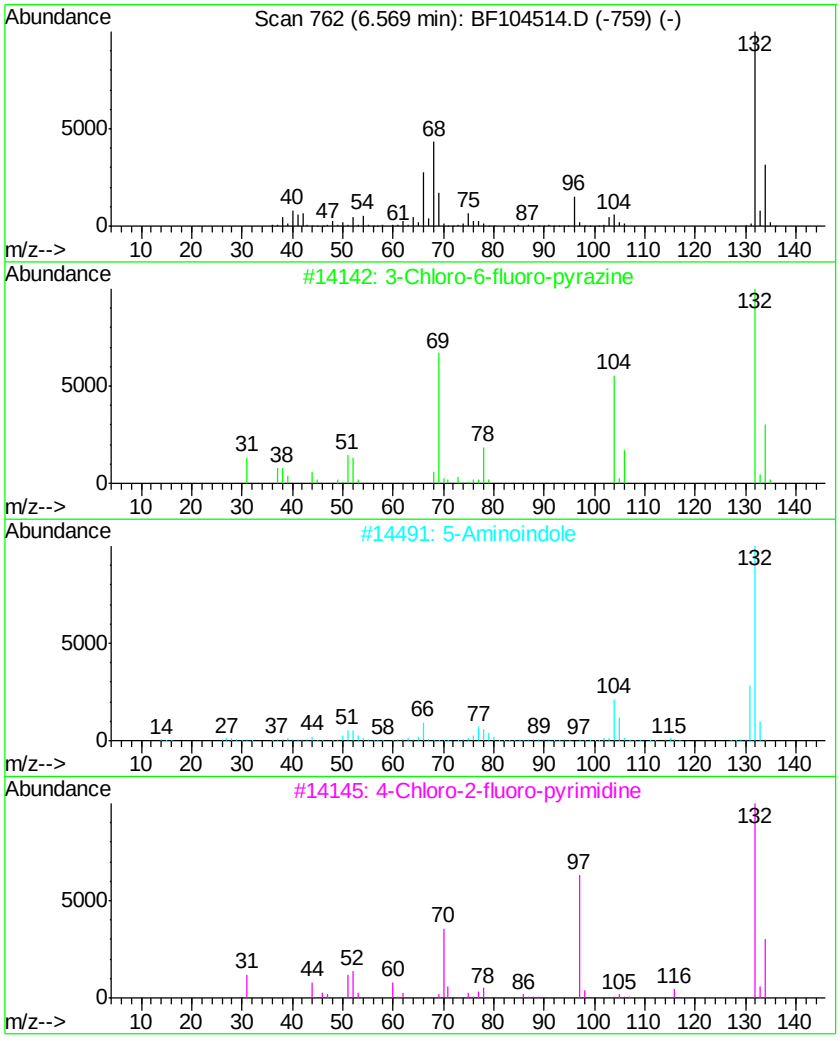
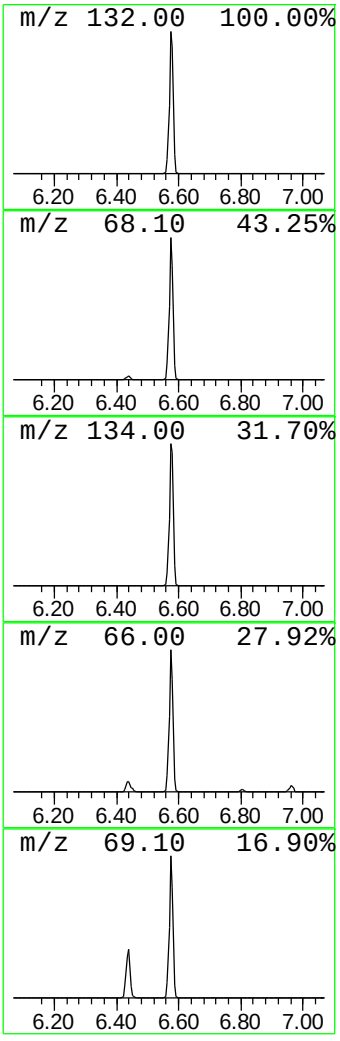
Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	52.41 ng	1803300	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Data File : BF104514.D
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Operator : JU/SJ
Sample : J2368-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRI-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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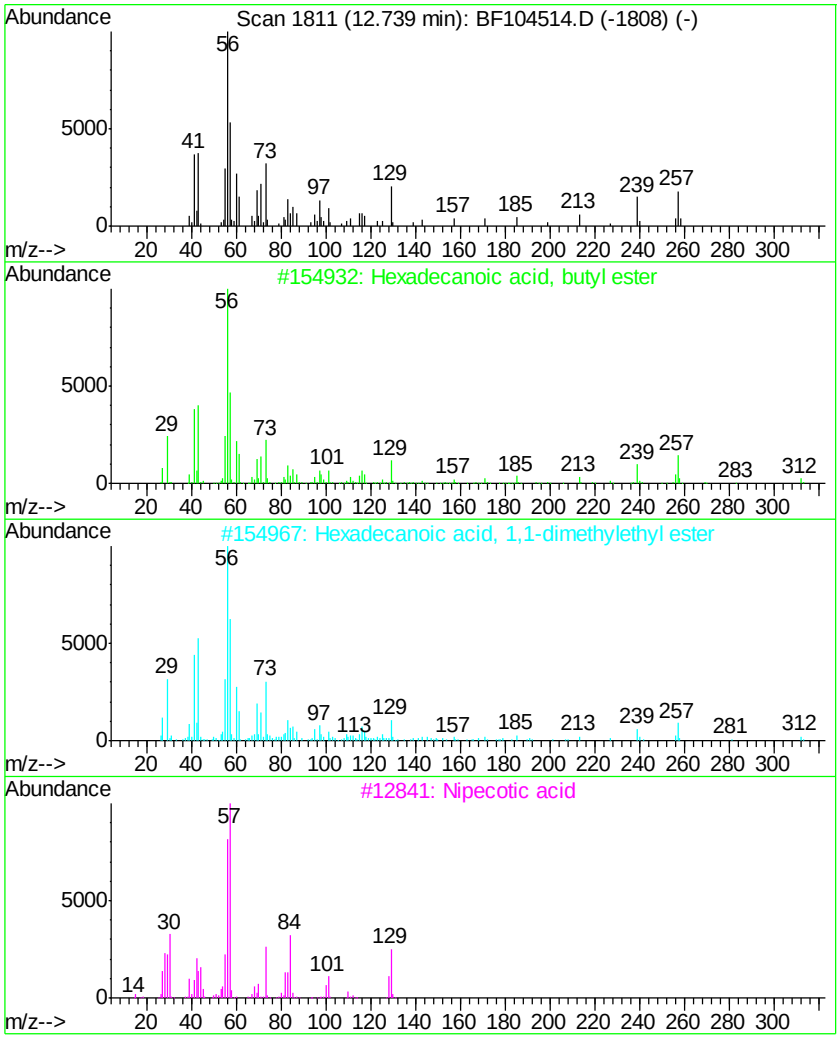
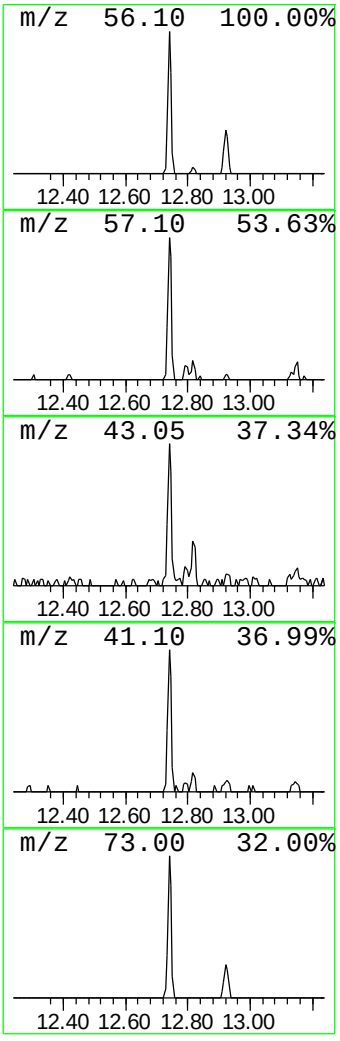
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.44 ng	103284	Chrysene-d12	13.98

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	Nipecotic acid	129	C6H11NO2	000498-95-3	50
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5	Cyclohexanamine	99	C6H13N	000108-91-8	30





Library Search Compound Report

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Sample : J2368-08
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-DBRI-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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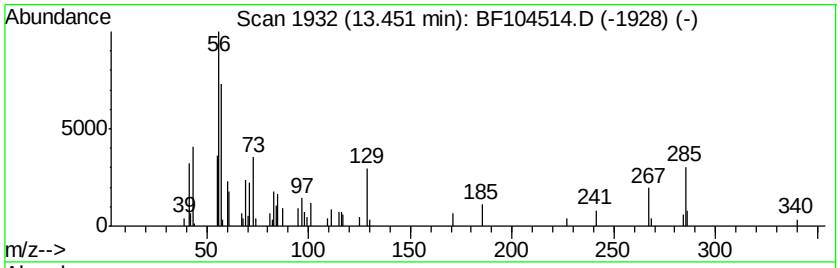
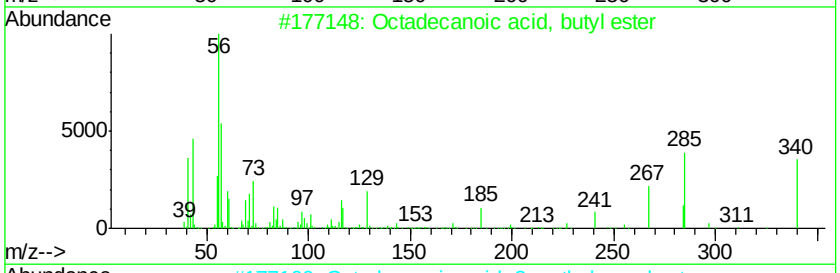
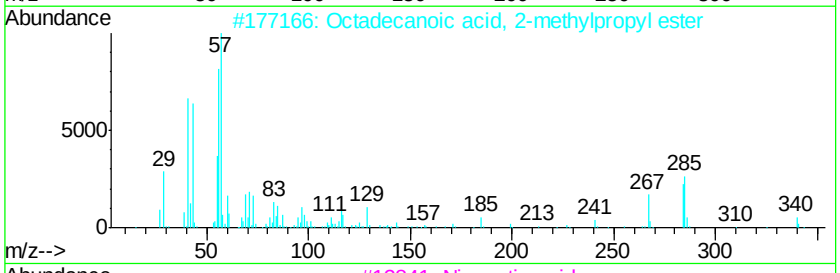
Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

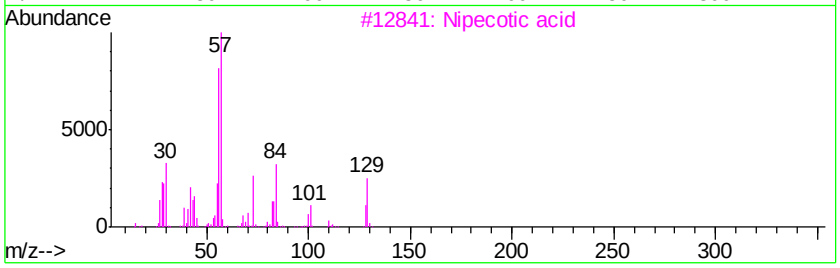
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	2.07 ng	62216	Chrysene-d12	13.98

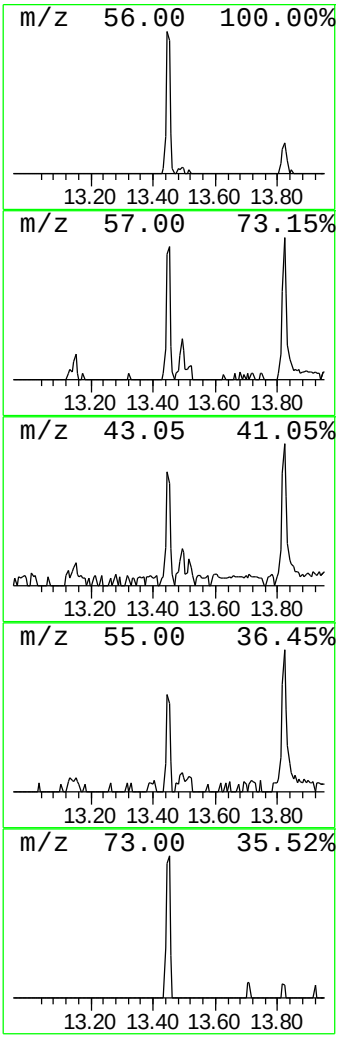
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	72
3	Nipecotic acid	129	C6H11NO2	000498-95-3	43
4	Butyl myristate	284	C18H36O2	000110-36-1	40
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	27











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

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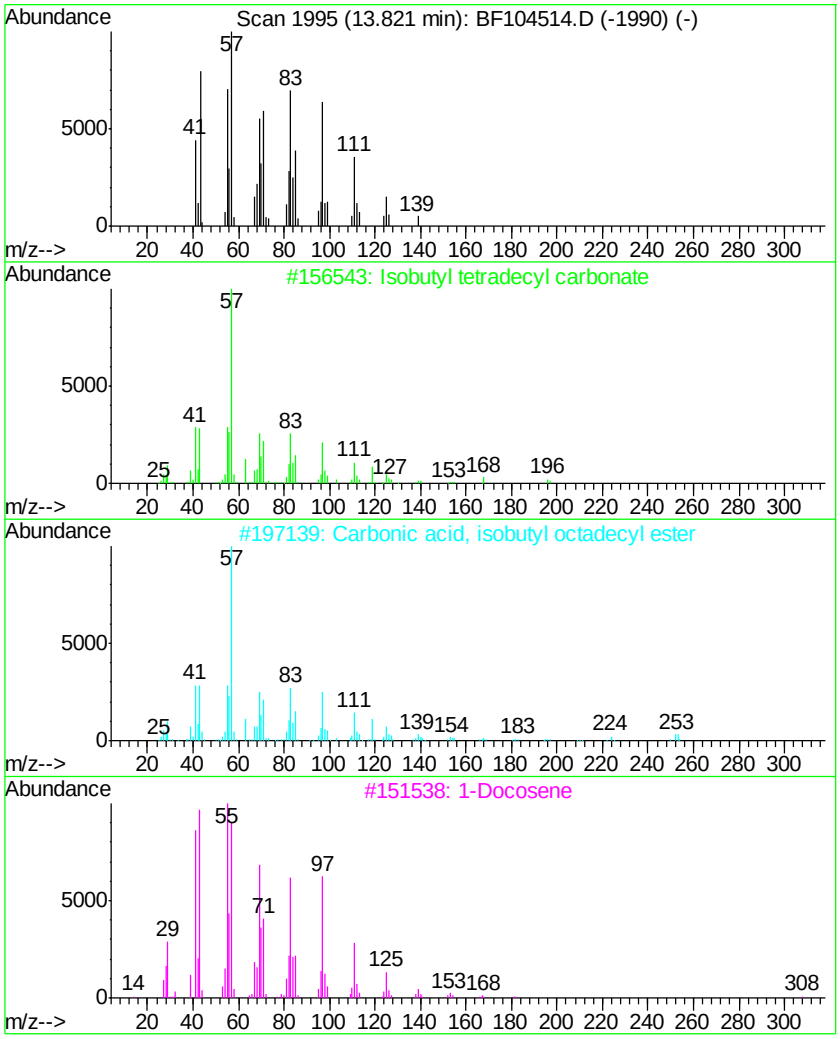
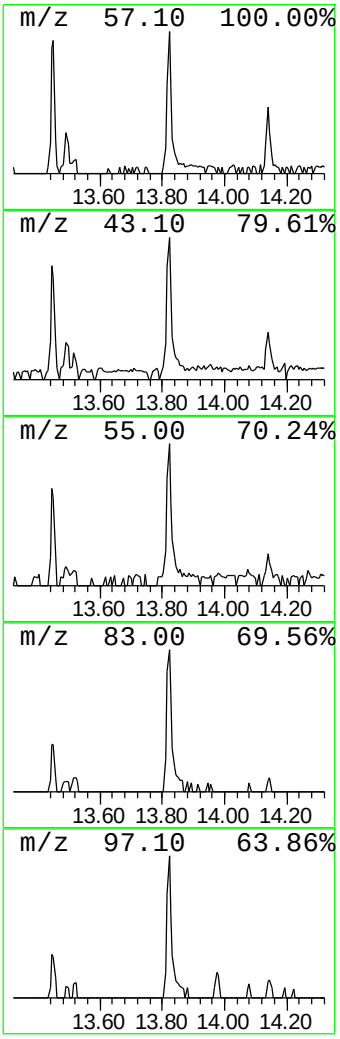
Peak Number 6 Isobutyl tetradecyl carbonate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.64 ng	79336	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	91
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91
3	1-Docosene	308	C22H44	001599-67-3	74
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	72
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	64





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
2-Pentanone, 4-hy...	5.00	2.7	ng	93911	1	6.81	688122	20.0
unknown6.57	6.57	52.4	ng	1803300	1	6.81	688122	20.0
Hexadecanoic acid...	12.74	3.4	ng	103284	5	13.98	600877	20.0
Octadecanoic acid...	13.45	2.1	ng	62216	5	13.98	600877	20.0
Isobutyl tetradec...	13.82	2.6	ng	79336	5	13.98	600877	20.0