LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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	2.192	16	18	28	rVB2	34610	59126	2.50%	0.278%
2	5.110	510	514	524	rBV	385825	474366	20.07%	2.227%
3	5.504	576	581	584	rBV	2315741	2246749	95.07%	10.546%
4	6.510	746	752	756	rBV	2107889	2321936	98.25%	10.899%
5	6.651	771	776	779	rBV	2434714	2262484	95.73%	10.620%
6	6.880	812	815	819	rBV	815107	714392	30.23%	3.353%
7	7.039	838	842	845	rBV	2085894	1786450	75.59%	8.385%
8	7.445	906	911	914	rBV	1592773	1423056	60.21%	6.679%
9	8.163	1029	1033	1037	rBV	1121612	928688	39.30%	4.359%
10	8.716	1124	1127	1130	rBV	84883	63576	2.69%	0.298%
11	9.239	1211	1216	1219	rBV	2697329	2363301	100.00%	11.093%
12	9.627	1278	1282	1285	rBV	171525	124459	5.27%	0.584%
13	9.916	1327	1331	1335	rBV	978592	923854	39.09%	4.336%
14	10.627	1448	1452	1455	rBV	156509	115869	4.90%	0.544%
15	10.704	1461	1465	1469	rBV	1370820	1179999	49.93%	5.539%
16	11.404	1580	1584	1587	rBV	931680	763604	32.31%	3.584%
17	11.915	1668	1671	1676	rBV	112008	114125	4.83%	0.536%
18	12.704	1801	1805	1811	rBV2	43389	48150	2.04%	0.226%
19	12.986	1849	1853	1856	rBV	1767298	1505369	63.70%	7.066%
20	13.868	2000	2003	2015	rBV	233284	277270	11.73%	1.301%
21	14.039	2028	2032	2036	rBV	802705	697132	29.50%	3.272%
22	14.503	2108	2111	2114	rBV5	21049	35571	1.51%	0.167%
23	14.656	2134	2137	2143	rVB	105592	121576	5.14%	0.571%
24	15.145	2218	2220	2225	rBV5	25360	30467	1.29%	0.143%
25	15.515	2278	2283	2291	rBV	573639	723405	30.61%	3.395%

Sum of corrected areas: 21304974

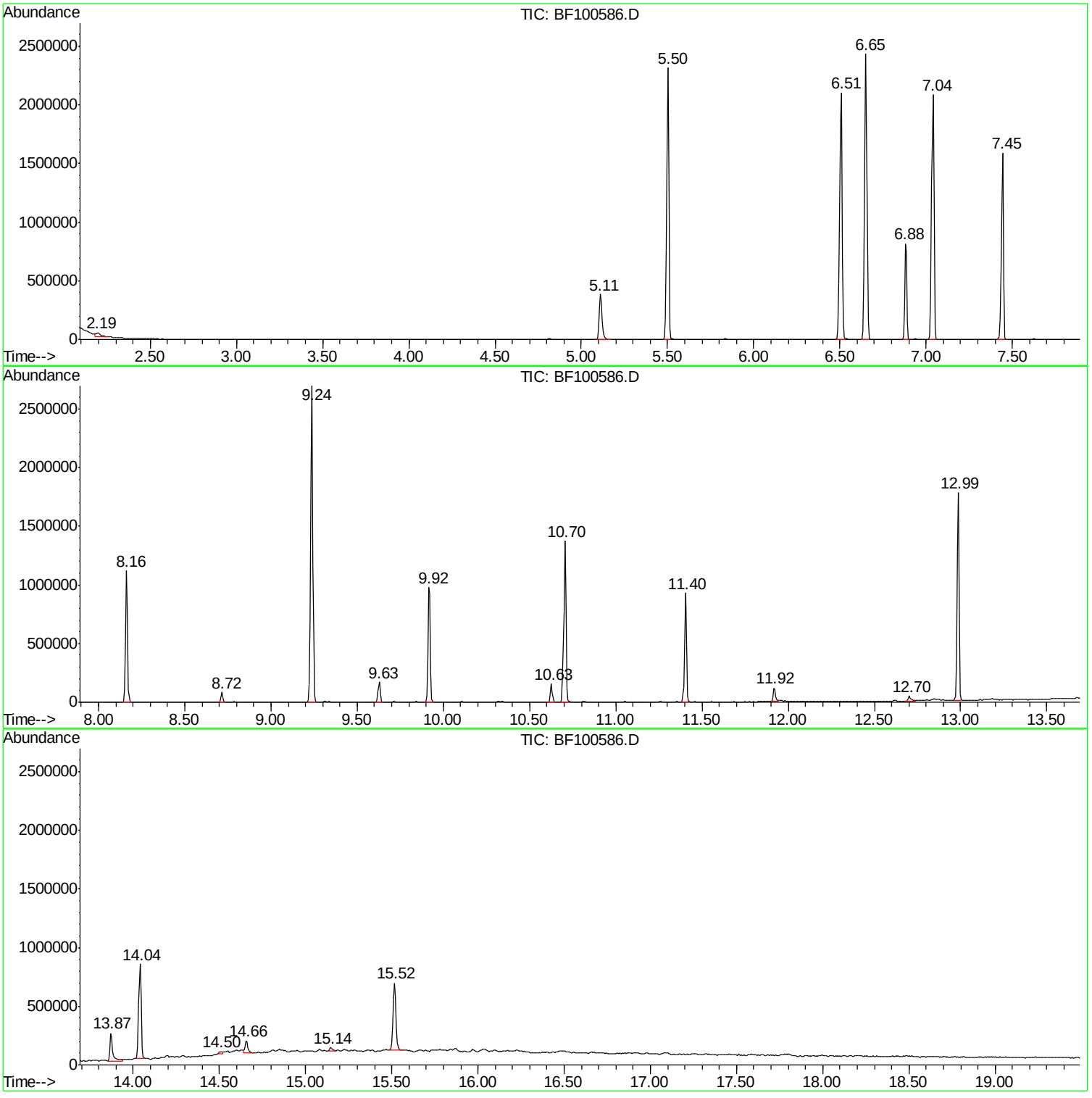
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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

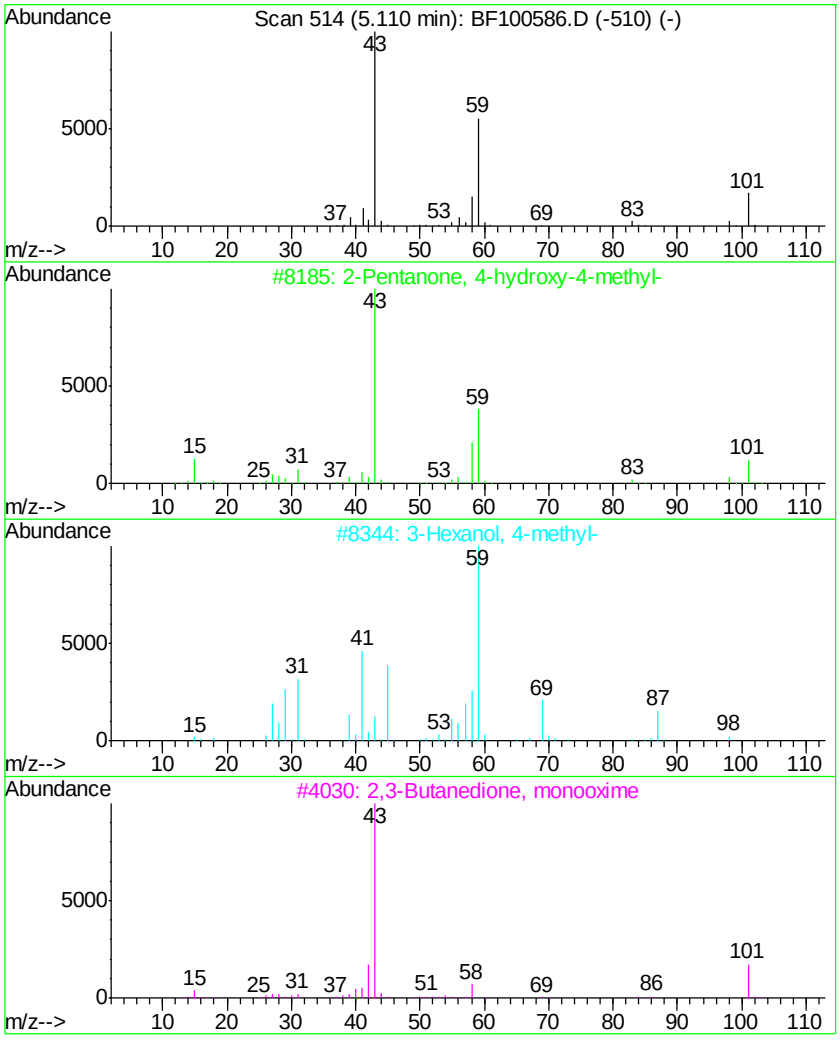
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

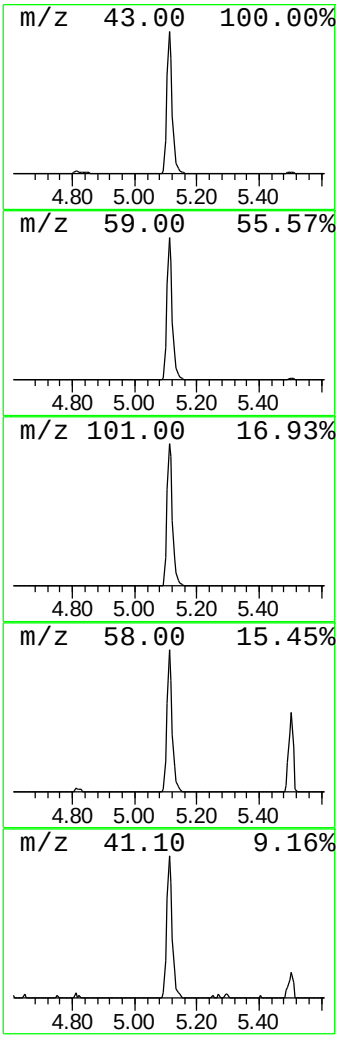
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	13.28 ng	474366	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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

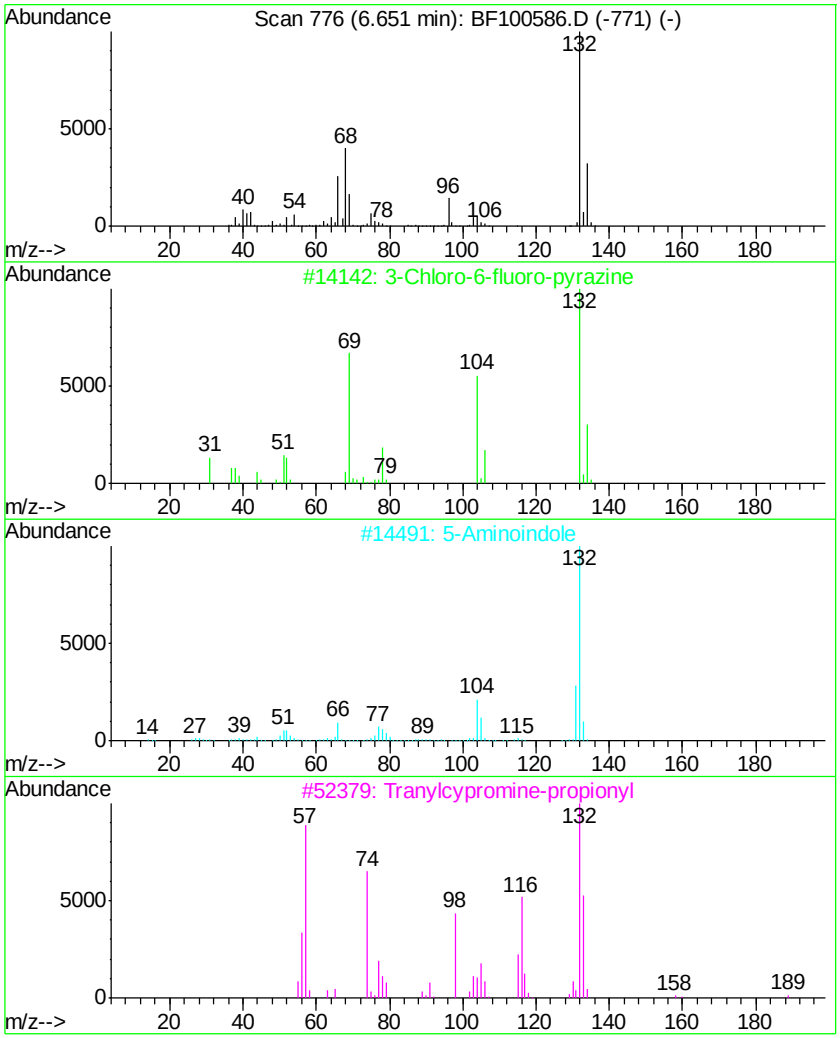
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

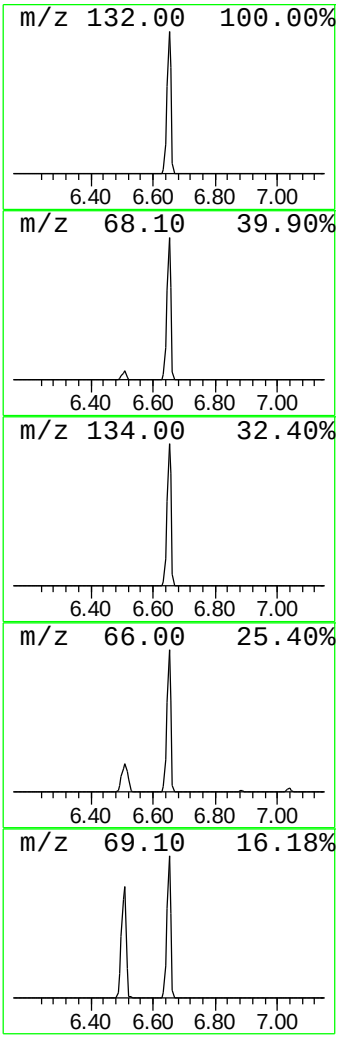
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	63.34 ng	2262480	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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

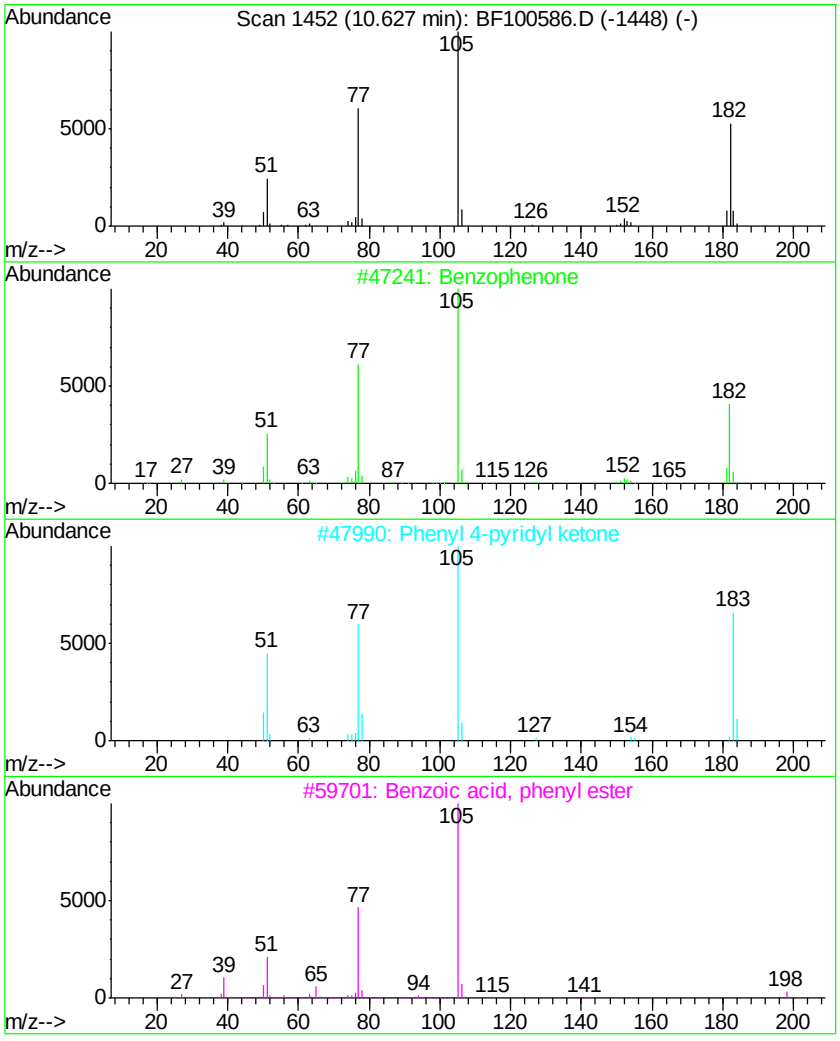
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

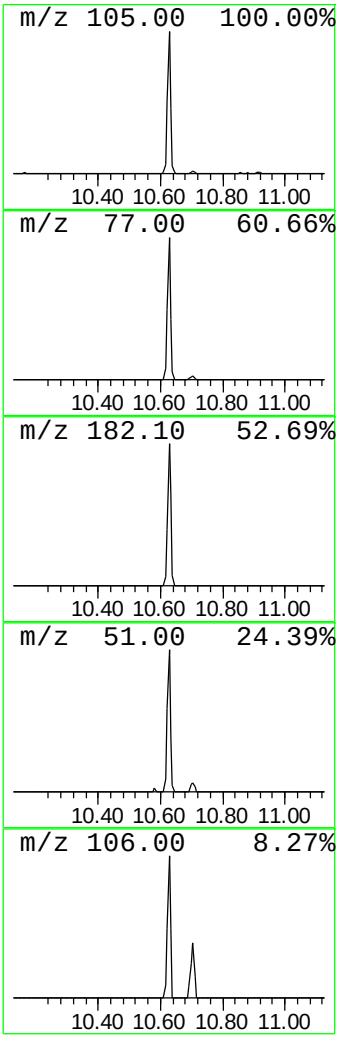
****

Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.51 ng	115869	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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

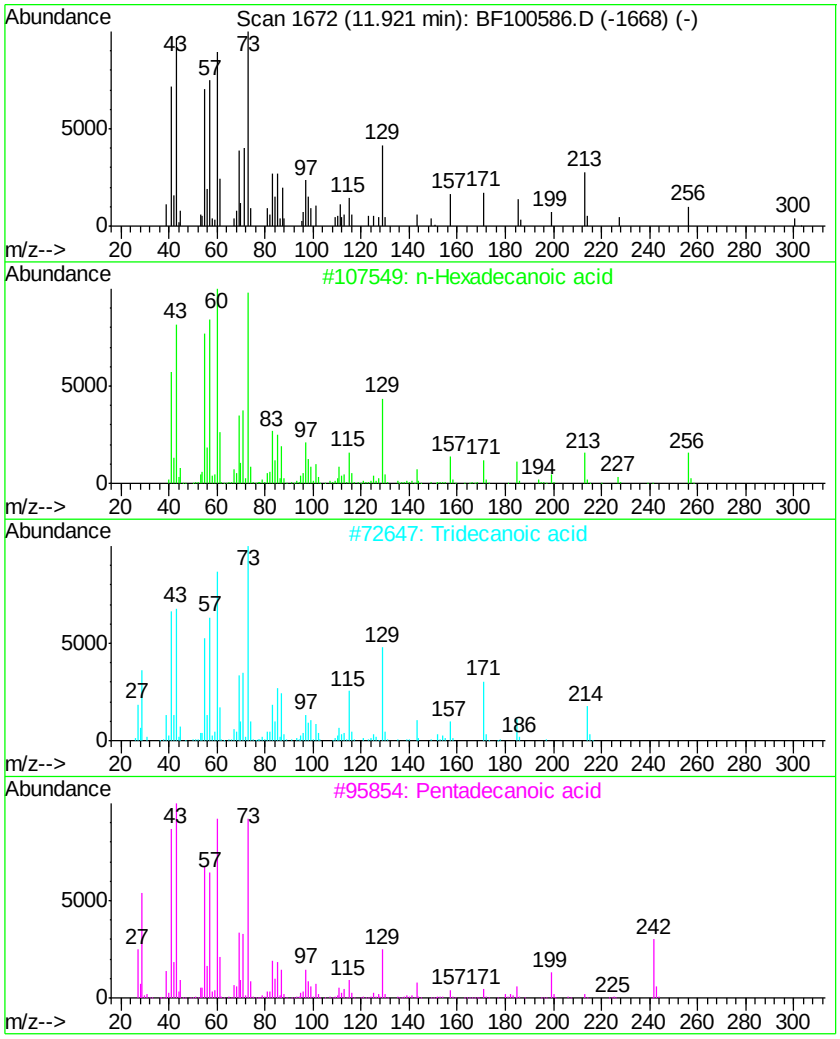
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

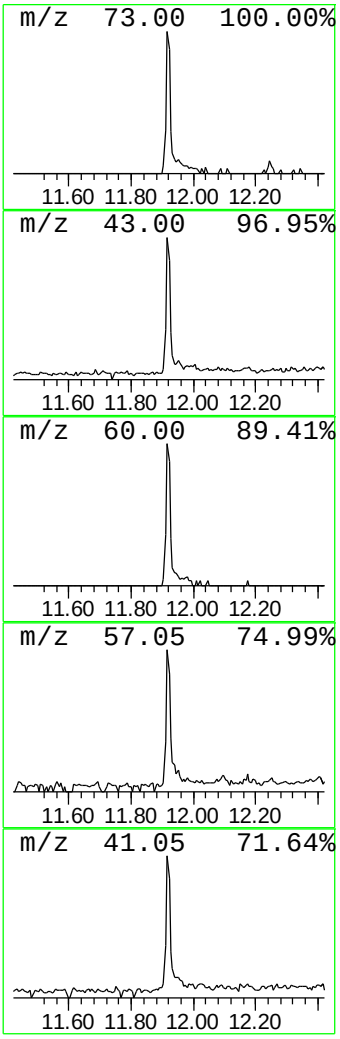
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.99 ng	114125	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	18





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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

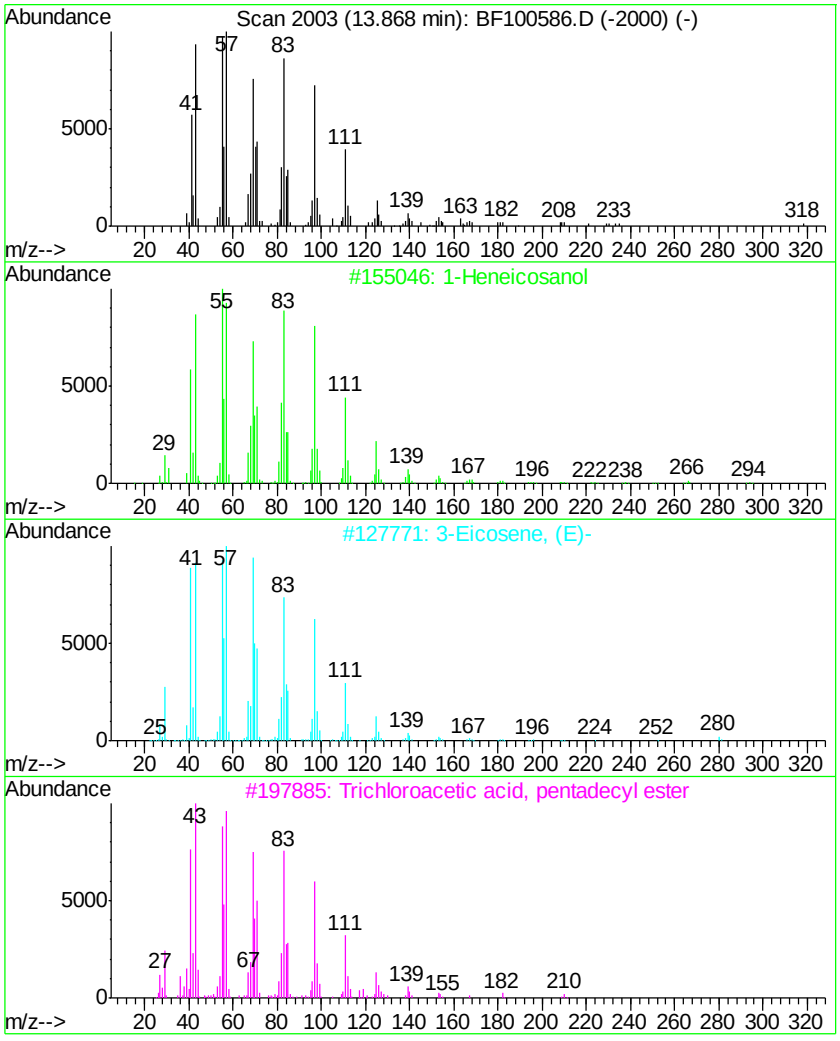
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

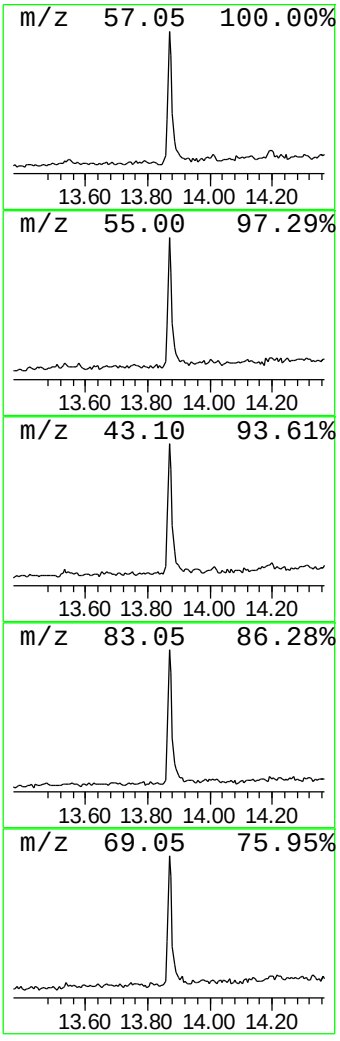
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	7.95 ng	277270	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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

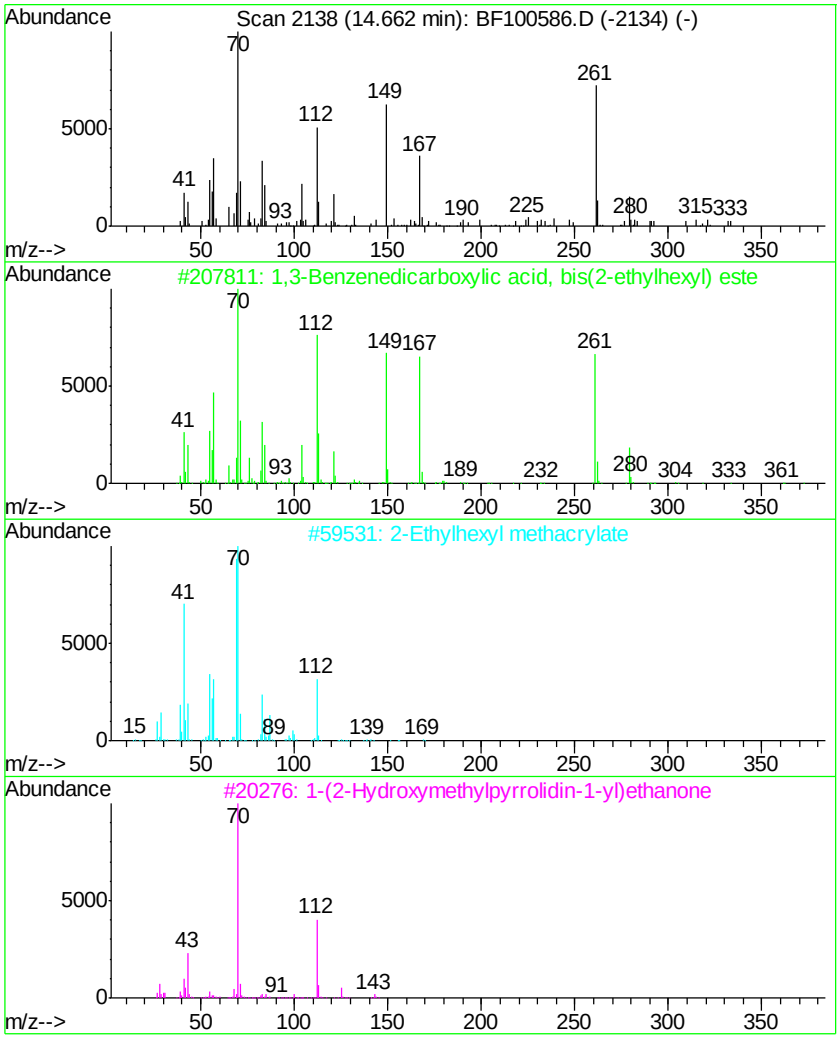
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

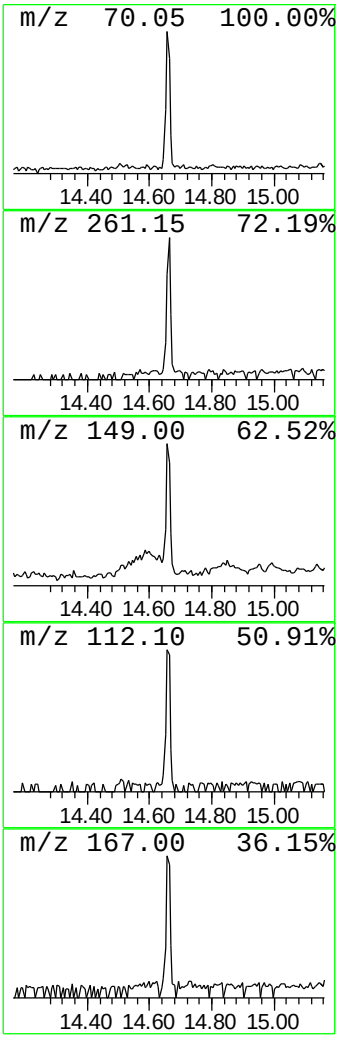
****

Peak Number 7 unknown14.66 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.49 ng	121576	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
2	2-Ethylhexyl methacrylate	198	C12H22O2	000688-84-6	25
3	1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	25
4	2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	25
5	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100586.D
Acq On : 15 Nov 2017 14:23
Operator : SJ/JU
Sample : I6441-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9A-9B

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
2-Pentanone, 4-hy...	5.11	13.3	ng	474366	1	6.88	714392	20.0
unknown6.65	6.65	63.3	ng	2262480	1	6.88	714392	20.0
Benzophenone	10.63	2.5	ng	115869	3	9.92	923854	20.0
n-Hexadecanoic acid	11.92	3.0	ng	114125	4	11.40	763604	20.0
1-Heneicosanol	13.87	8.0	ng	277270	5	14.04	697132	20.0
unknown14.66	14.66	3.5	ng	121576	5	14.04	697132	20.0