LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

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-BF030717.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	4.904	262	264	277	rBV	216555	428729	8.40%	1.011%
2	5.350	301	303	316	rBV	1663325	2727597	53.41%	6.432%
3	5.750	335	338	346	rVB2	35704	60980	1.19%	0.144%
4	6.402	394	395	403	rBV2	1315878	1961373	38.41%	4.625%
5	6.516	403	405	408	rBV	3397382	4179337	81.84%	9.855%
6	6.744	423	425	428	rBV	1162592	1174332	23.00%	2.769%
7	6.904	436	439	441	rBV	4193993	3988947	78.11%	9.406%
8	6.996	445	447	454	rVB3	42907	92361	1.81%	0.218%
9	7.270	467	471	473	rBV3	33212	61539	1.21%	0.145%
10	7.327	473	476	478	rBV	3257249	3813765	74.68%	8.993%
11	7.613	499	501	505	rBV2	74322	96013	1.88%	0.226%
12	7.716	507	510	517	rVV	405857	595392	11.66%	1.404%
13	7.842	519	521	524	rVB	55841	91746	1.80%	0.216%
14	7.967	529	532	535	rVB3	56417	131207	2.57%	0.309%
15	8.036	535	538	540	rBV	1783579	1647870	32.27%	3.886%
16	8.379	566	568	570	rBV2	34254	66468	1.30%	0.157%
17	8.470	574	576	579	rVV	420076	452598	8.86%	1.067%
18	8.562	582	584	587	rVV	141219	137651	2.70%	0.325%
19	8.779	600	603	607	rVB3	49465	84969	1.66%	0.200%
20	8.893	612	613	619	rVB4	51814	86626	1.70%	0.204%
21	8.996	619	622	624	rBV2	66292	167024	3.27%	0.394%
22	9.065	626	628	629	rBV	86524	83033	1.63%	0.196%
23	9.110	629	632	634	rVV	5433884	5106723	100.00%	12.042%
24	9.168	634	637	638	rVB2	41909	61074	1.20%	0.144%
25	9.293	644	648	650	rBV3	76612	153048	3.00%	0.361%
26	9.328	650	651	653	rVV2	53512	65489	1.28%	0.154%
27	9.430	657	660	661	rBV3	69738	121841	2.39%	0.287%
28	9.510	665	667	669	rVB	156257	169135	3.31%	0.399%
29	9.602	673	675	677	rBV3	54024	100148	1.96%	0.236%
30	9.716	683	685	688	rBV3	50901	82594	1.62%	0.195%
31	9.785	688	691	693	rBV	1884856	1715022	33.58%	4.044%
32	9.968	703	707	709	rVB5	44833	89652	1.76%	0.211%
33	10.025	711	712	716	rBV2	105262	153001	3.00%	0.361%
34	10.116	718	720	722	rVV	415441	464035	9.09%	1.094%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

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-BF030717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.208	727	728	733	rVV	177160	235124	4.60%	0.554%
36	10.310	735	737	739	rVV2	42797	67445	1.32%	0.159%
37	10.356	739	741	744	rVV2	72274	101435	1.99%	0.239%
38	10.425	745	747	751	rVB3	86616	163216	3.20%	0.385%
39	10.585	758	761	763	rBV	2186960	2843183	55.68%	6.705%
40	10.688	768	770	774	rVB2	140762	191616	3.75%	0.452%
41	11.133	807	809	811	rBV2	115868	110819	2.17%	0.261%
42	11.271	819	821	823	rBV	1735438	1508837	29.55%	3.558%
43	11.556	844	846	852	rBV3	43001	94404	1.85%	0.223%
44	11.739	860	862	864	rBV3	53791	67448	1.32%	0.159%
45	11.808	867	868	875	rVB2	134187	194850	3.82%	0.459%
46	12.859	957	960	962	rBV	3535411	4199774	82.24%	9.904%
47	13.751	1036	1038	1044	rBV	110533	147839	2.89%	0.349%
48	13.911	1050	1052	1055	rVB	1142729	1034081	20.25%	2.438%
49	15.317	1172	1175	1181	rVB	790782	1035217	20.27%	2.441%

Sum of corrected areas: 42406607

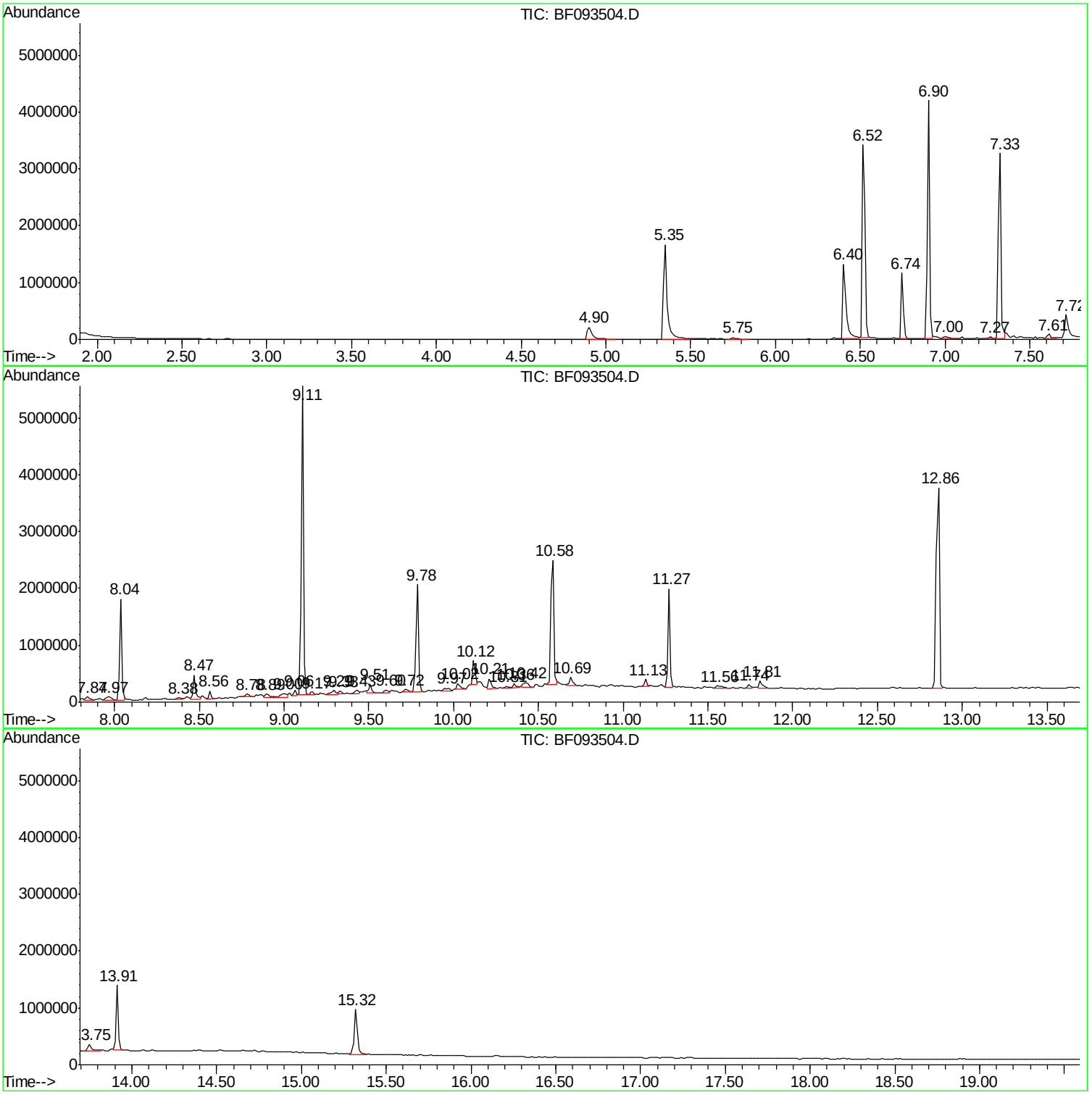
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

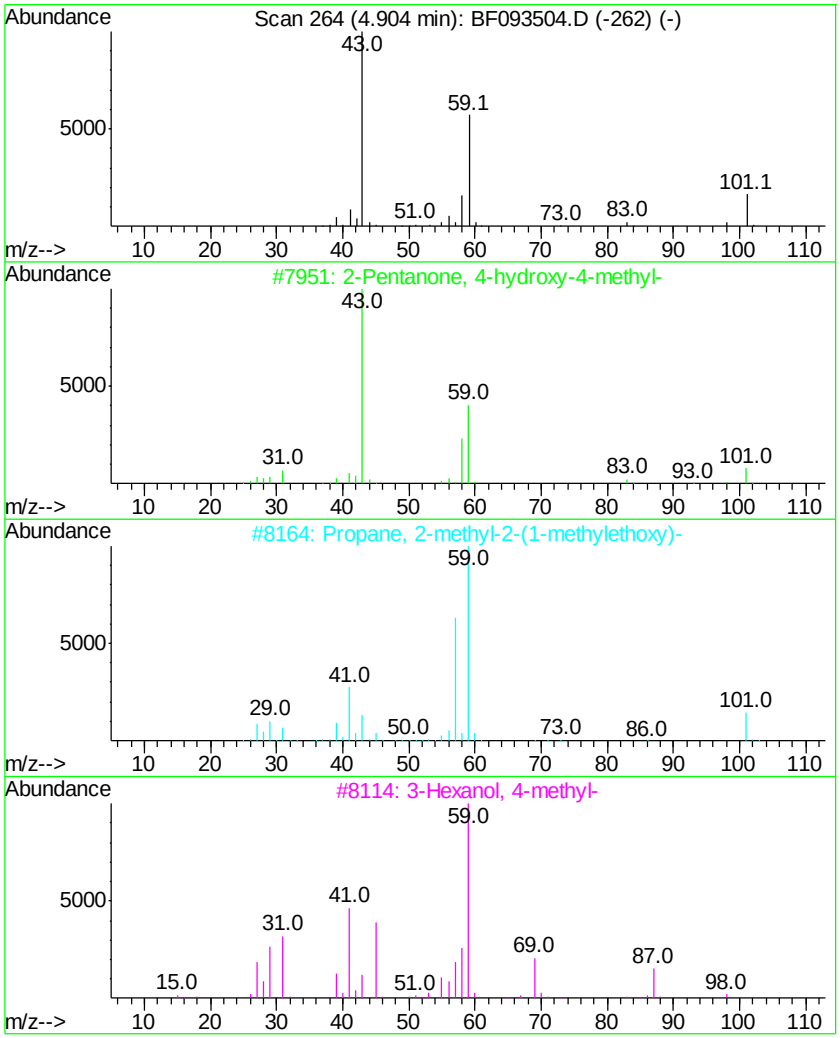
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

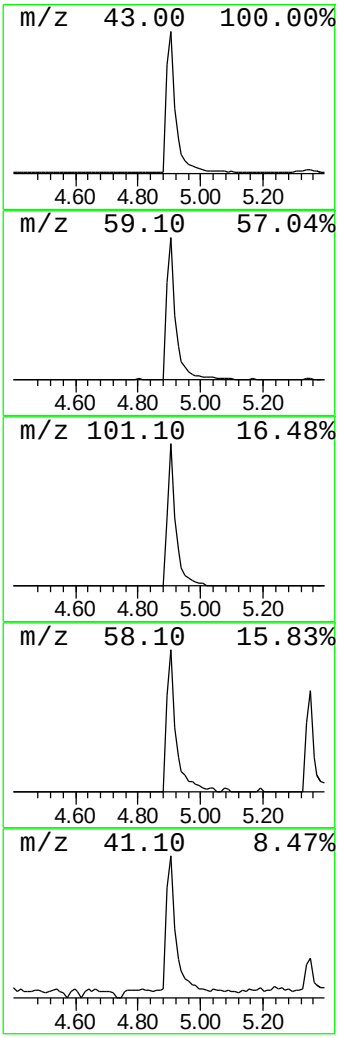
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	7.30 ng	428729	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

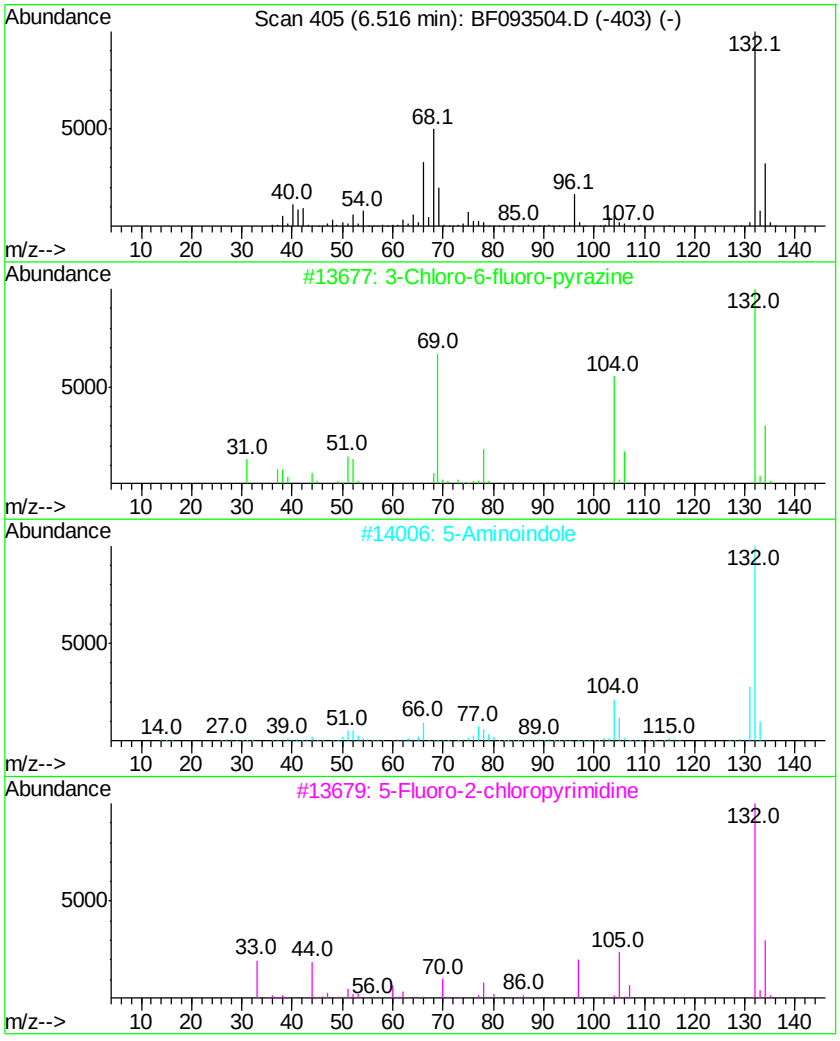
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

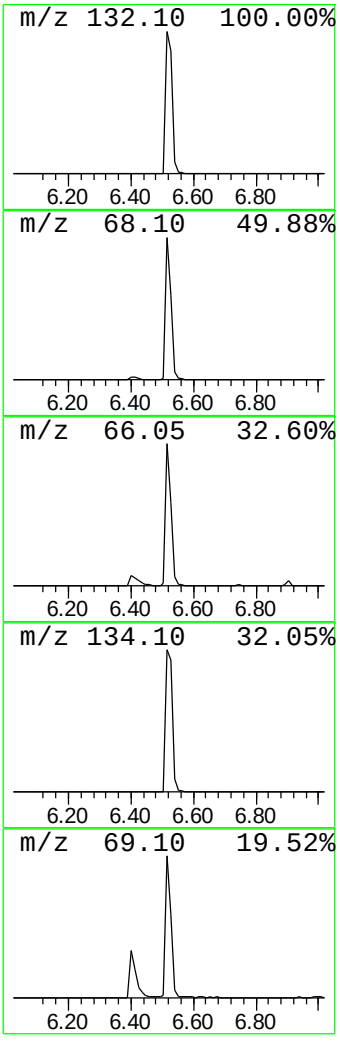
****

Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	71.18 ng	4179340	1,4-Dichlorobenzene-d4	6.74

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	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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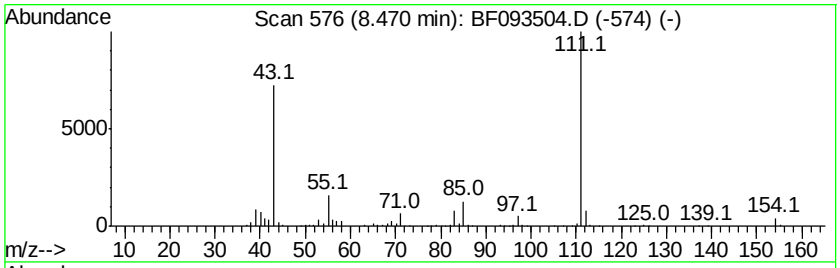
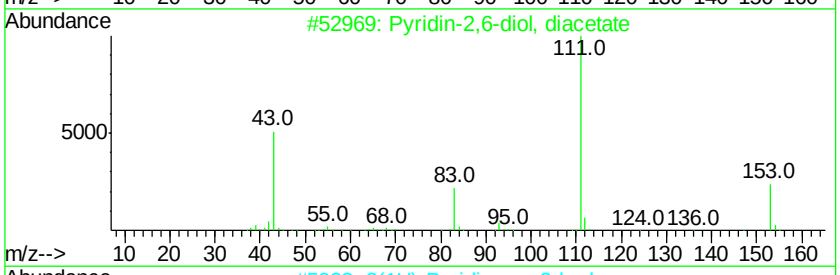
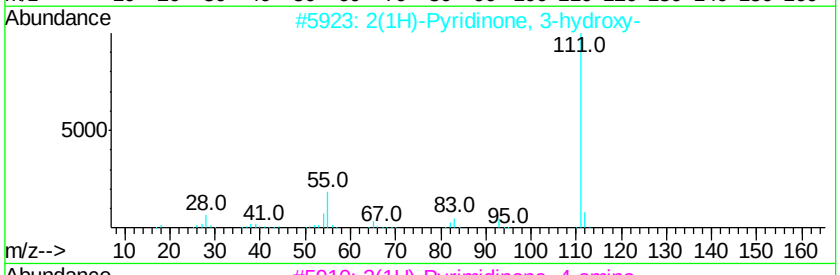
Peak Number 4 unknown8.47 Concentration Rank 4

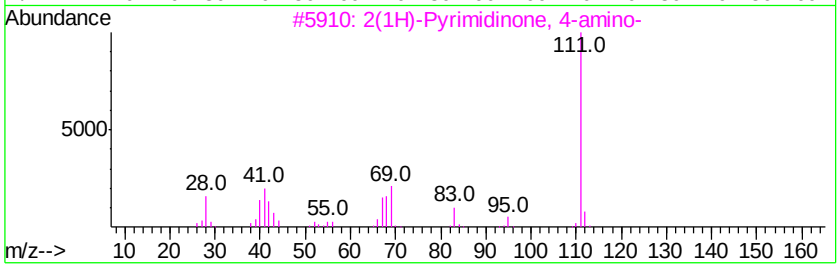
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	5.49 ng	452598	Naphthalene-d8	8.04

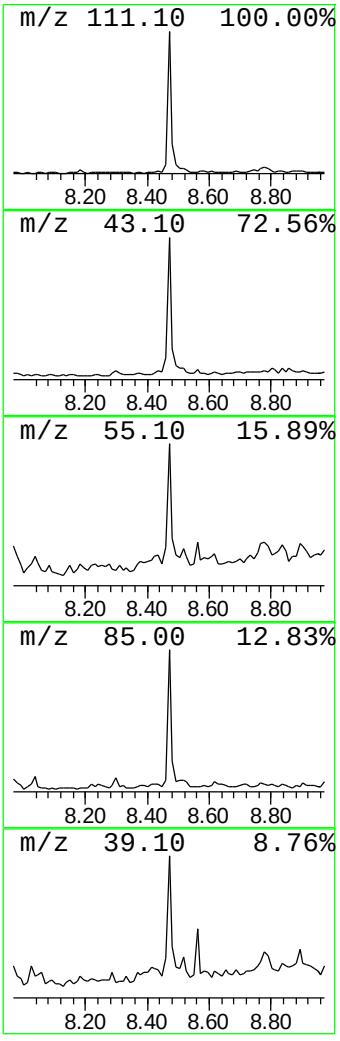
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridin-2,6-diol, diacetate	195	C9H9NO4	1000153-09-2	45
2	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	42
3	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	36
4	4-Amino-6-hydroxypyrimidine	111	C4H5N3O	001193-22-2	9
5	3-Aminopyrazine 1-oxide	111	C4H5N3O	006863-77-0	9











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Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
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Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

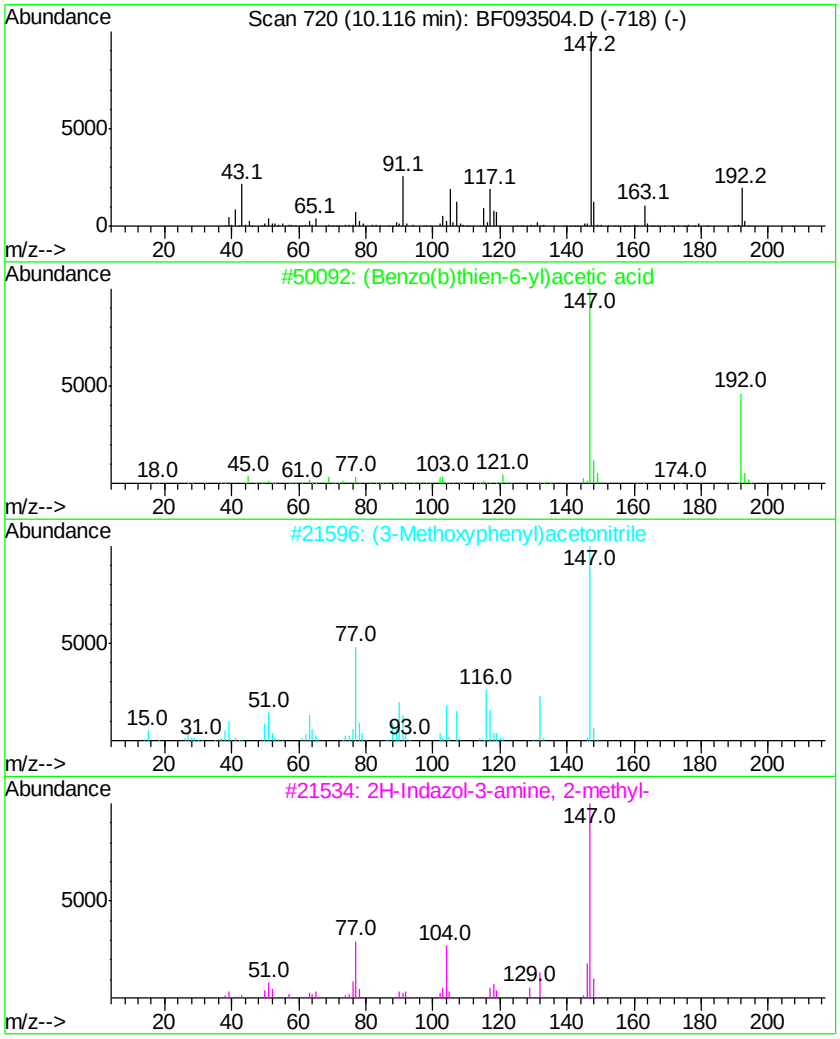
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

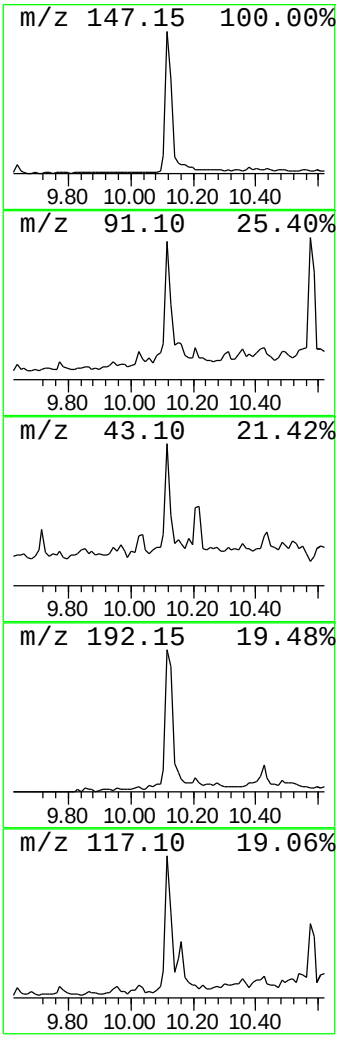
****

Peak Number 5 unknown10.12 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.12	5.41 ng	464035	Acenaphthene-d10	9.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Benzo(b)thien-6-yl)acetic acid	192	C10H8O2S	006177-87-3	47
2	(3-Methoxyphenyl)acetonitrile	147	C9H9NO	019924-43-7	47
3	2H-Indazol-3-amine, 2-methyl-	147	C8H9N3	097990-19-7	43
4	Benzoic acid, 4-propyl-, 4-cyano...	265	C17H15NO2	056131-49-8	43
5	Benzoyl chloride, 4-propyl-	182	C10H11ClO	052710-27-7	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

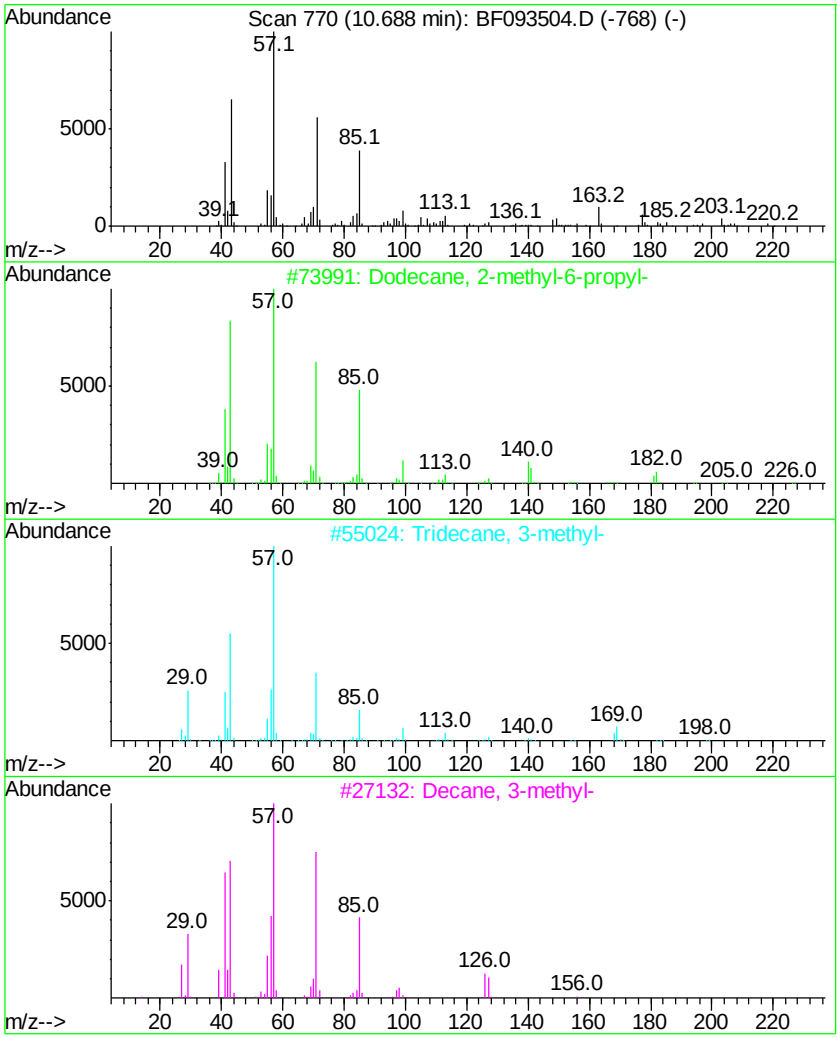
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

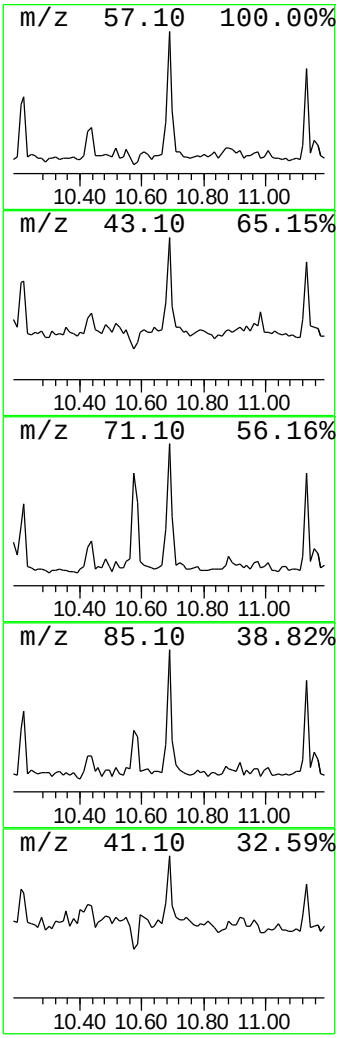
****

Peak Number 7 Dodecane, 2-methyl-6-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	2.54 ng	191616	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	64
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	59
3	Decane, 3-methyl-	156	C11H24	013151-34-3	59
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	59
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	50





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Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
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Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

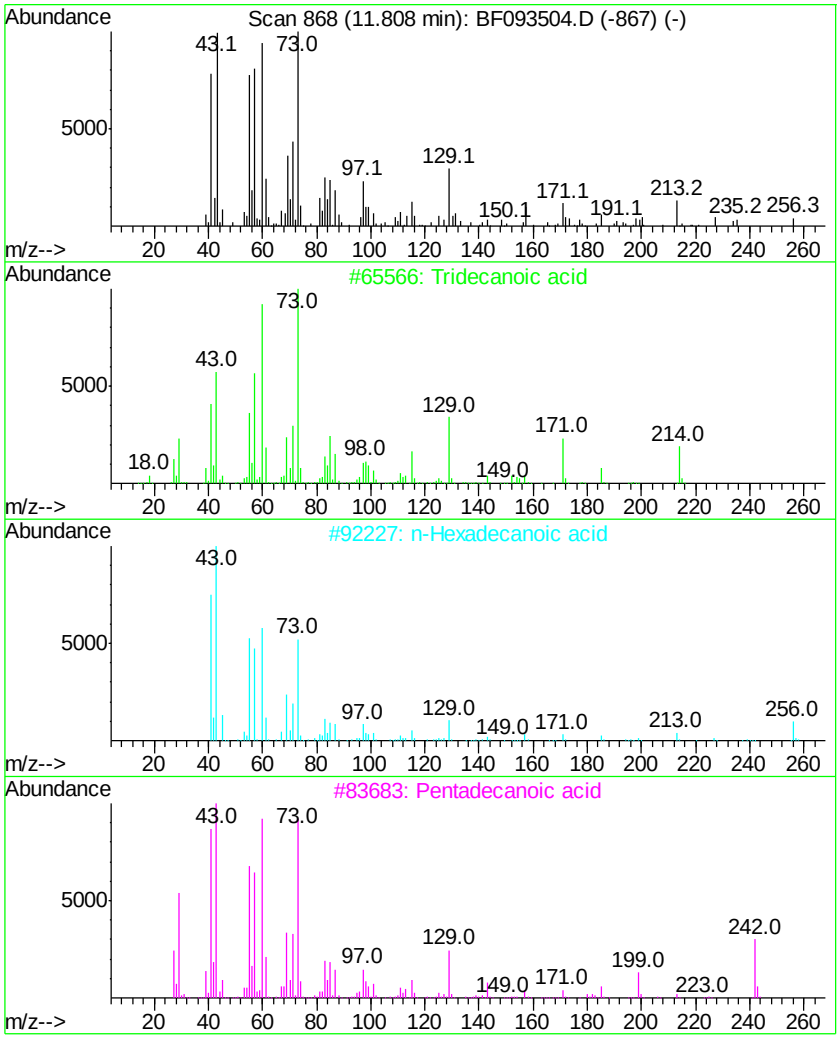
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

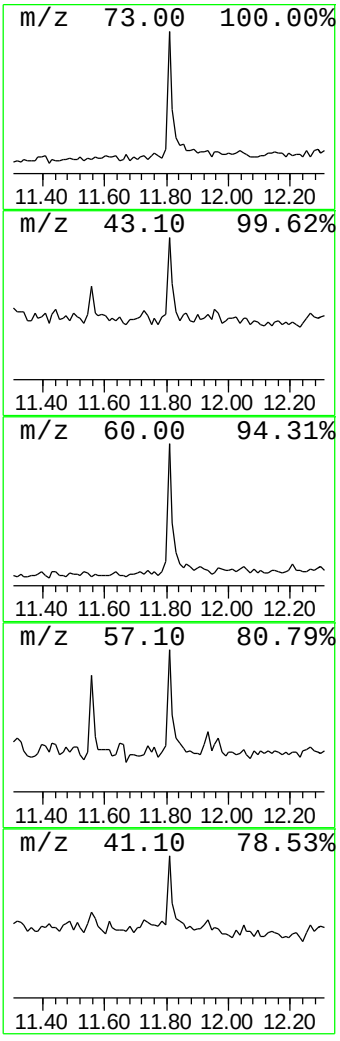
****

Peak Number 8 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	2.58 ng	194850	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Dodecanoic acid	200	C12H24O2	000143-07-7	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

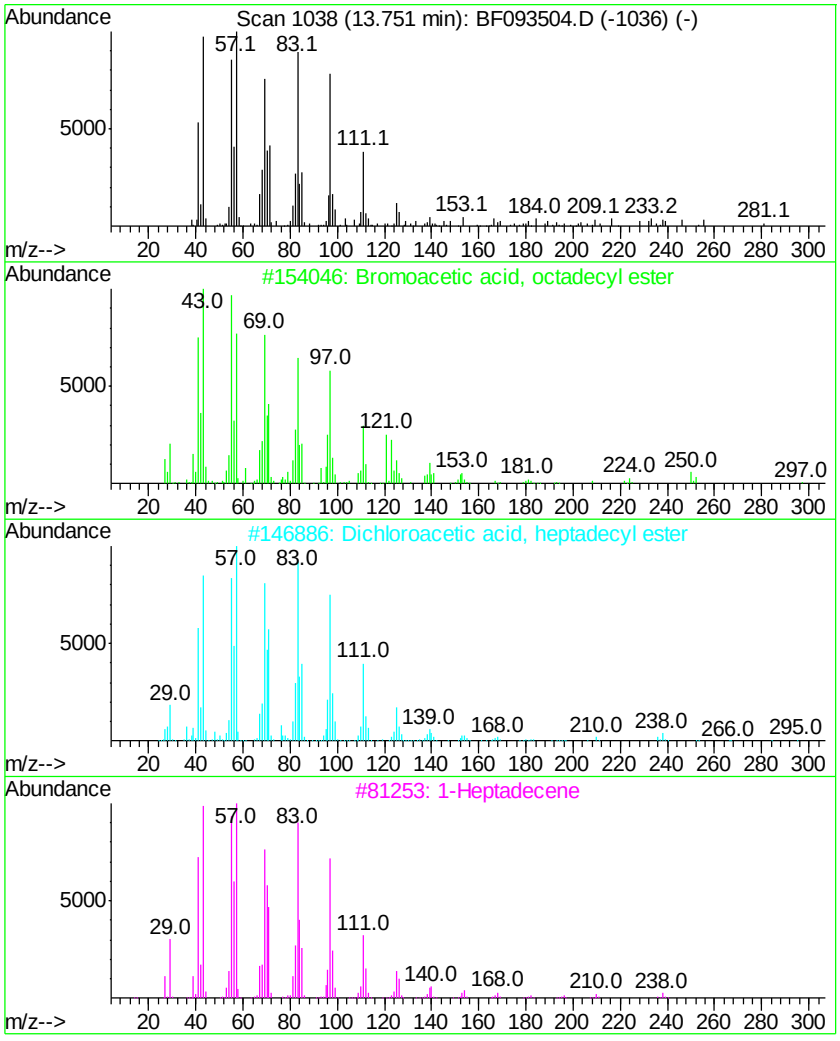
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

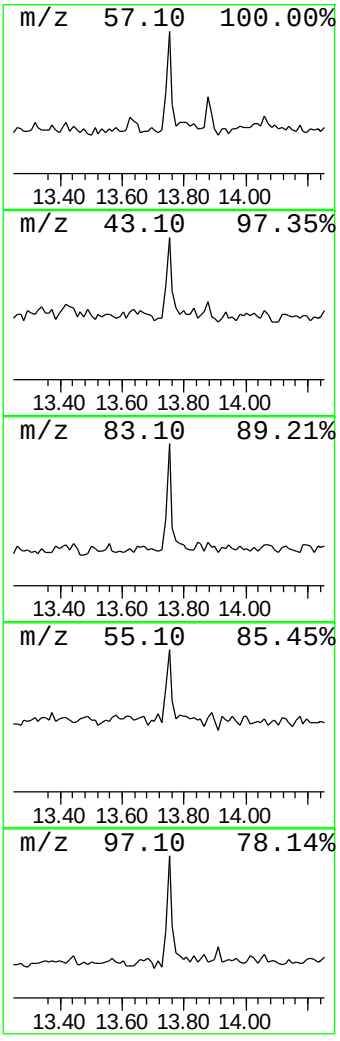
****

Peak Number 9 Bromoacetic acid, octadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	2.86 ng	147839	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3	1-Heptadecene	238	C17H34	006765-39-5	89
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87
5	E-14-Hexadecenal	238	C16H30O	330207-53-9	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030917\
Data File : BF093504.D
Acq On : 10 Mar 2017 4:31
Operator : SJ/MA
Sample : I2176-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-19

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	7.3	ng	428729	1	6.74	1174330	20.0
unknown6.52	6.52	71.2	ng	4179340	1	6.74	1174330	20.0
unknown8.47	8.47	5.5	ng	452598	2	8.04	1647870	20.0
unknown10.12	10.12	5.4	ng	464035	3	9.78	1715020	20.0
Dodecane, 2-methy...	10.69	2.5	ng	191616	4	11.27	1508840	20.0
Tridecanoic acid	11.81	2.6	ng	194850	4	11.27	1508840	20.0
Bromoacetic acid,...	13.75	2.9	ng	147839	5	13.91	1034080	20.0