LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092245.D
Acq On : 13 Jan 2017 13:18
Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SW-003

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-BF122116.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	4.724	253	257	271	rBV	1660233	3183481	48.77%	6.137%
2	5.193	295	298	300	rBV	4764724	6527940	100.00%	12.585%
3	6.256	388	391	394	rBV	4888077	6002531	91.95%	11.572%
4	6.359	398	400	403	rVV	5658460	6278833	96.18%	12.104%
5	6.587	418	420	422	rBV	1141835	1130626	17.32%	2.180%
6	6.747	431	434	436	rBV	3602220	4597690	70.43%	8.863%
7	7.159	467	470	473	rBV	3183035	3544370	54.30%	6.833%
8	7.867	530	532	535	rBV	1103715	1430373	21.91%	2.757%
9	8.953	624	627	630	rBV	5709678	5792882	88.74%	11.167%
10	9.353	660	662	664	rBV	1177266	980251	15.02%	1.890%
11	9.616	683	685	687	rBV	1176525	1338651	20.51%	2.581%
12	10.073	723	725	726	rVB	85412	79283	1.21%	0.153%
13	10.416	752	755	757	rBV	2230589	3064731	46.95%	5.908%
14	10.542	764	766	769	rBV	126895	154225	2.36%	0.297%
15	10.988	803	805	806	rBV	85633	83872	1.28%	0.162%
16	11.102	812	815	819	rVB2	799947	1258551	19.28%	2.426%
17	11.651	861	863	866	rVV2	222543	213244	3.27%	0.411%
18	12.302	918	920	922	rVB	202003	176147	2.70%	0.340%
19	12.531	937	940	942	rVV	148172	175956	2.70%	0.339%
20	12.679	951	953	956	rVB	2735037	3347985	51.29%	6.454%
21	13.594	1031	1033	1042	rBV	166230	313038	4.80%	0.603%
22	13.720	1042	1044	1047	rBV	874932	1020793	15.64%	1.968%
23	14.714	1129	1131	1135	rBV	68286	145594	2.23%	0.281%
24	15.034	1156	1159	1161	rBV	52778	68121	1.04%	0.131%
25	15.080	1161	1163	1166	rBV	703429	877098	13.44%	1.691%
26	15.548	1201	1204	1208	rBV4	29483	86476	1.32%	0.167%

Sum of corrected areas: 51872742

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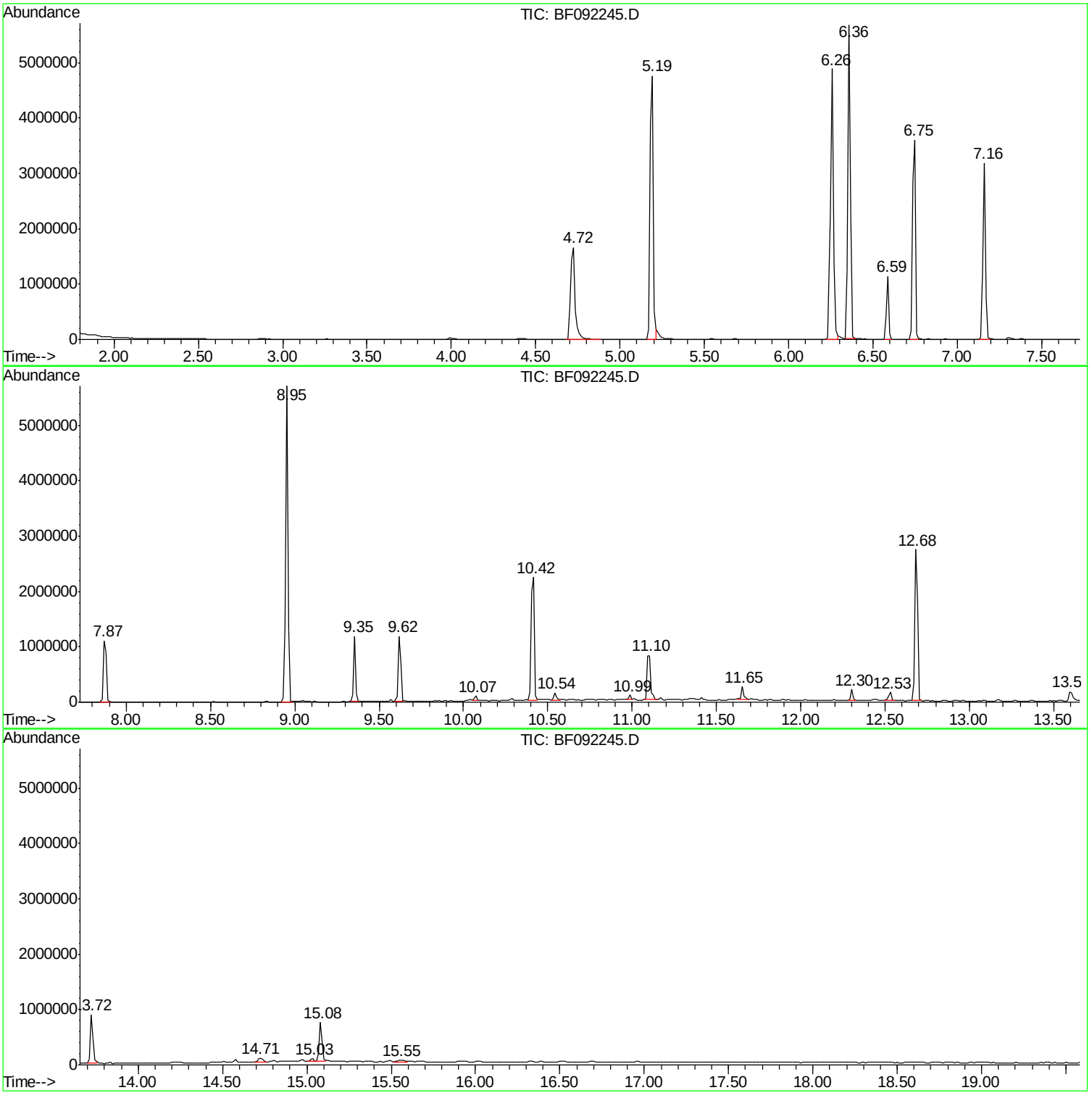
Instrument : BNA_F
ClientSampleId : SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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Data File : BF092245.D
Acq On : 13 Jan 2017 13:18
Operator : UM/SJ
Sample : I1131-06
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Instrument : BNA_F
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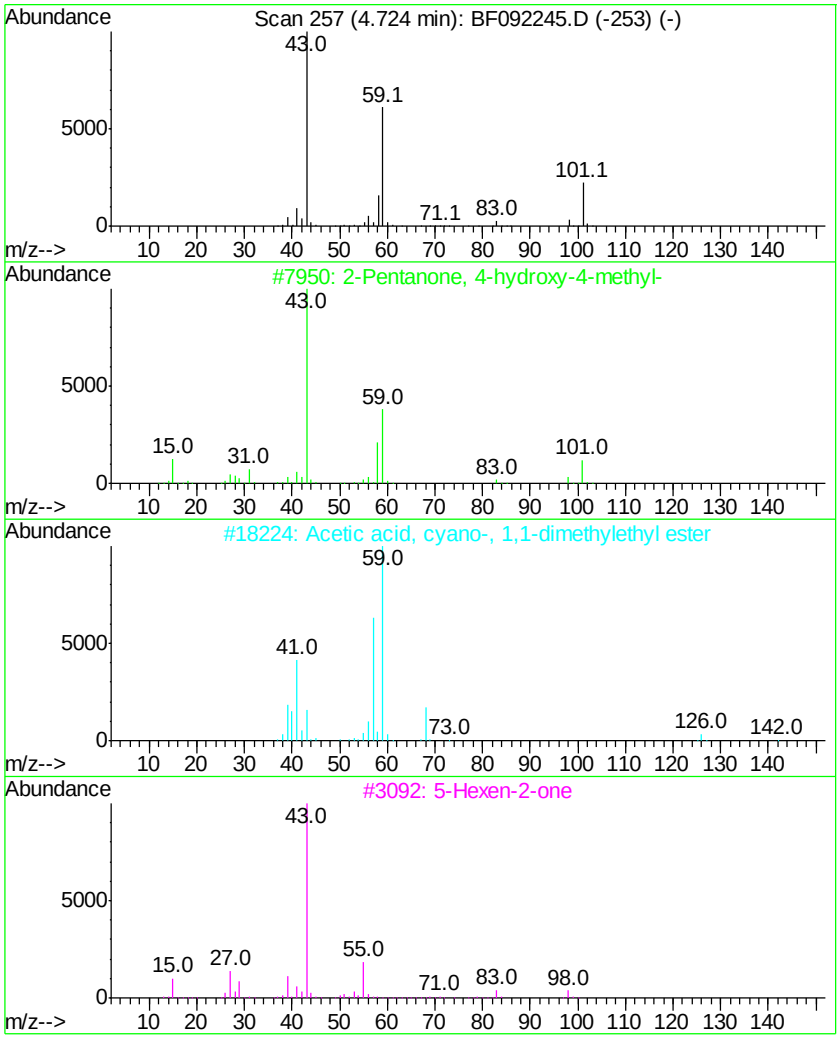
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

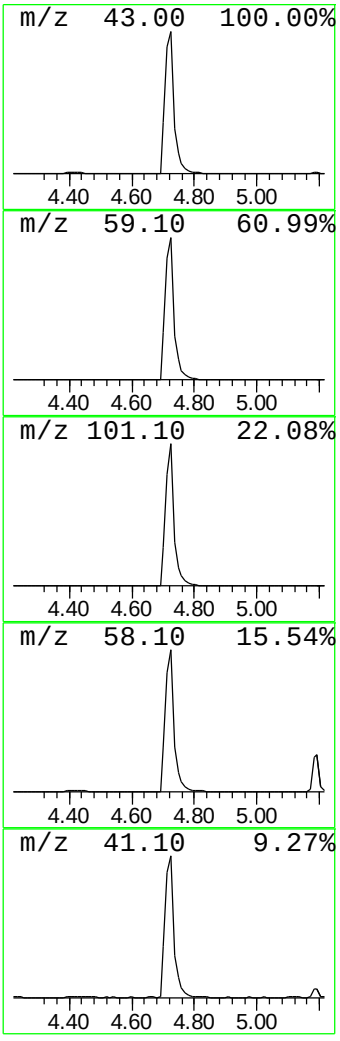
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	56.31 ng	3183480	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : I1131-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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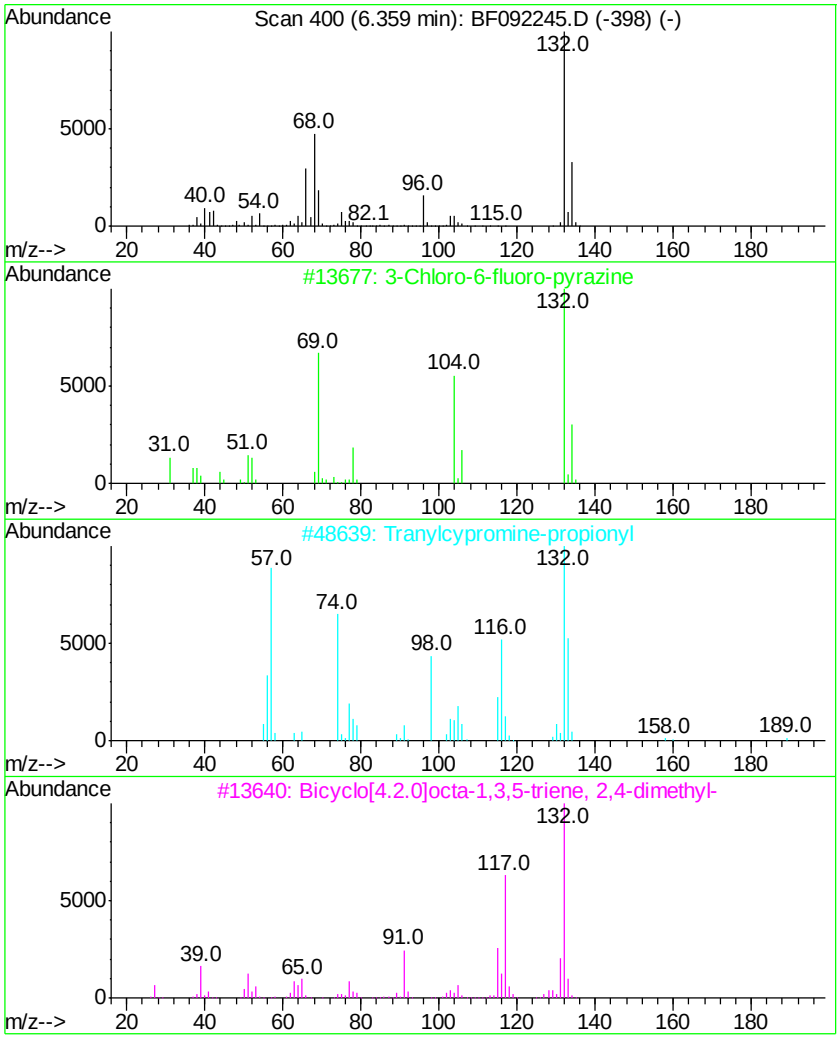
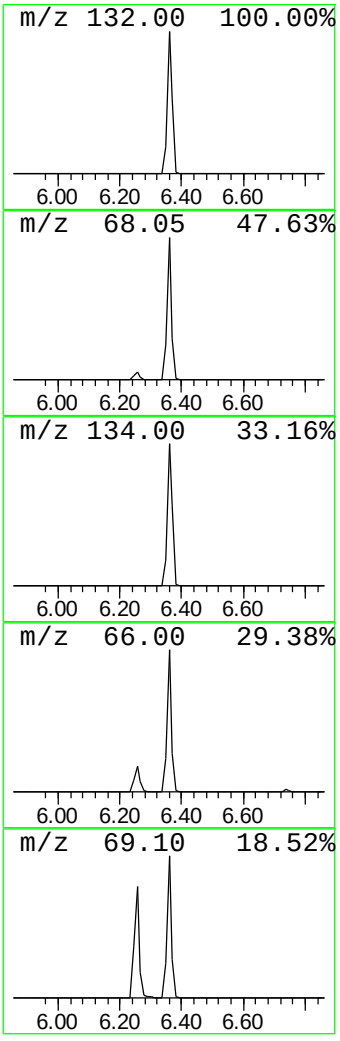
Peak Number 2 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	111.07 ng	6278830	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092245.D
Acq On : 13 Jan 2017 13:18
Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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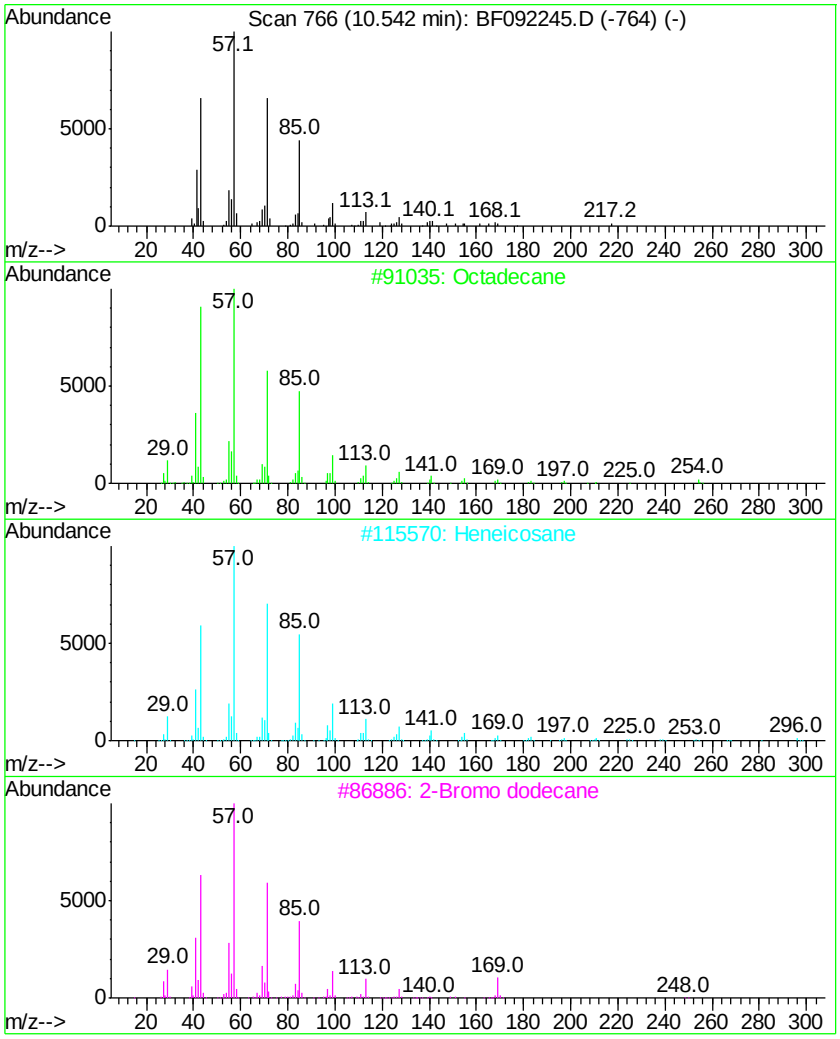
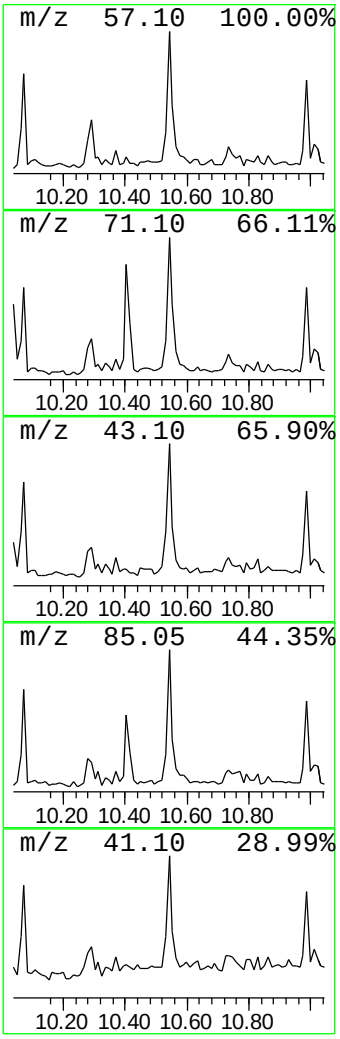
Peak Number 3 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	2.45 ng	154225	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Pentadecane	212	C15H32	000629-62-9	90





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Sample : I1131-06
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Instrument : BNA_F
ClientSampleId : SW-003

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

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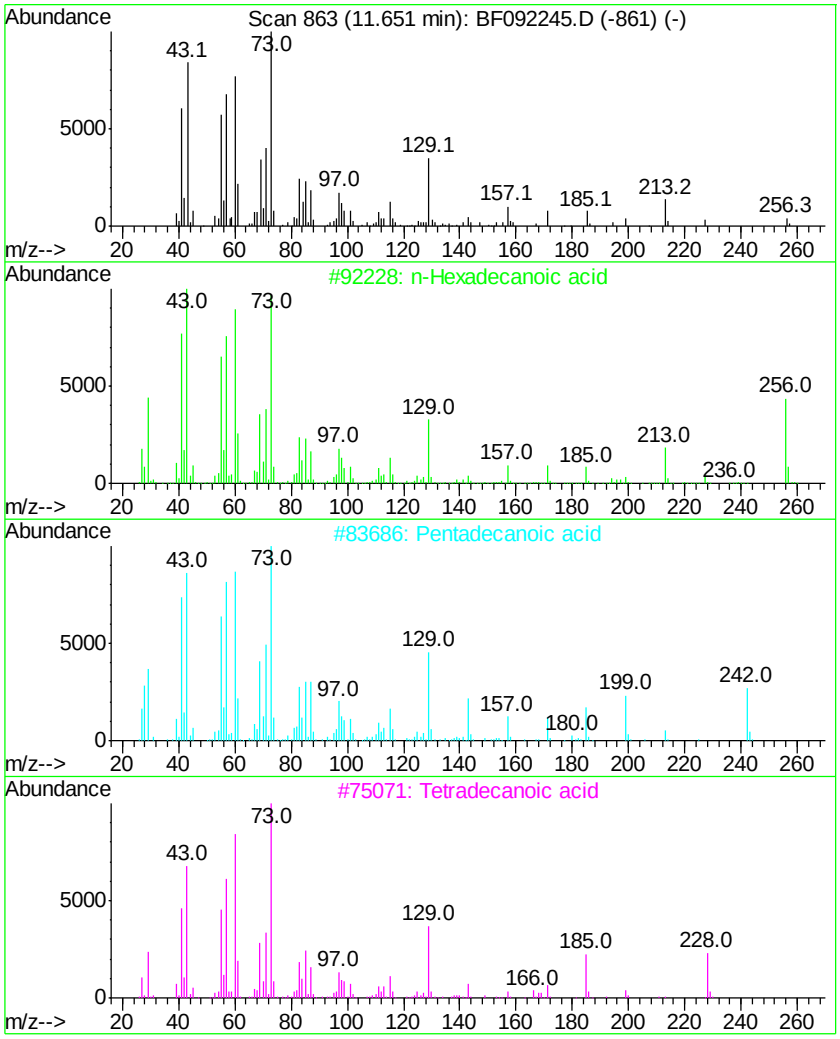
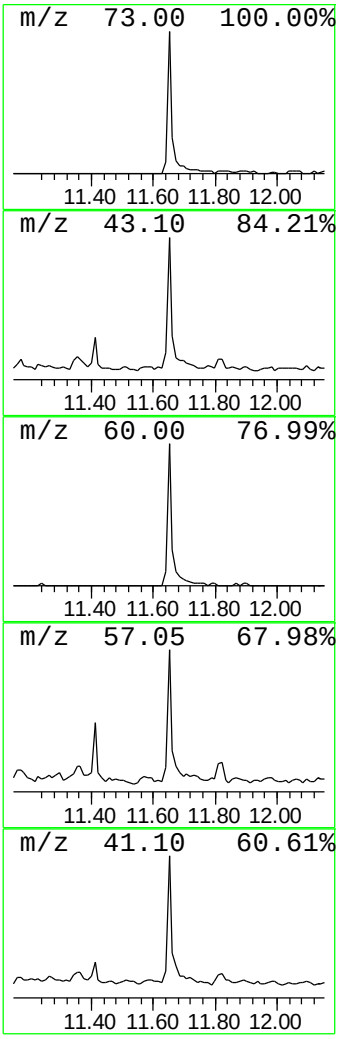
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	3.39 ng	213244	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	18





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Operator : UM/SJ
Sample : I1131-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SW-003

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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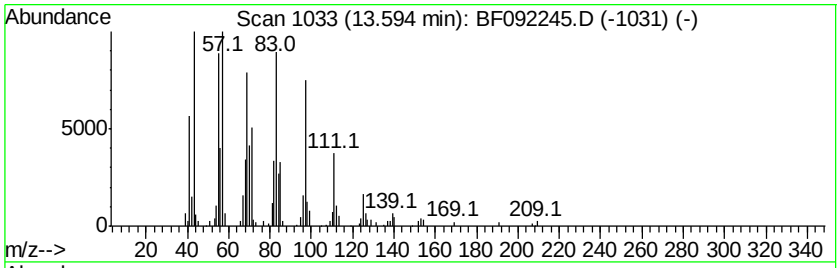
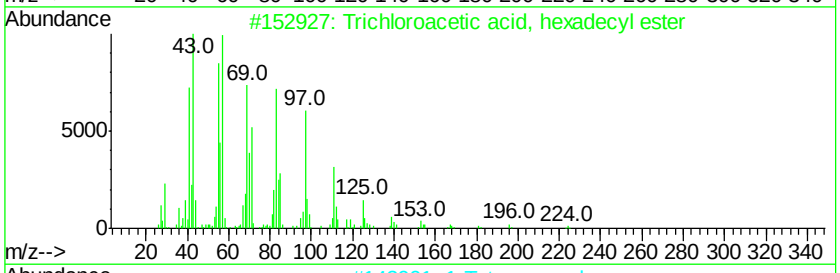
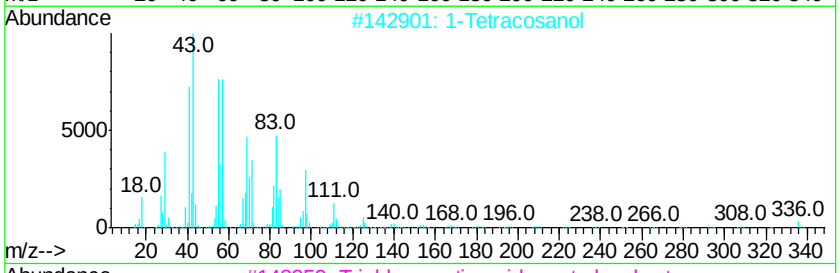
Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 3

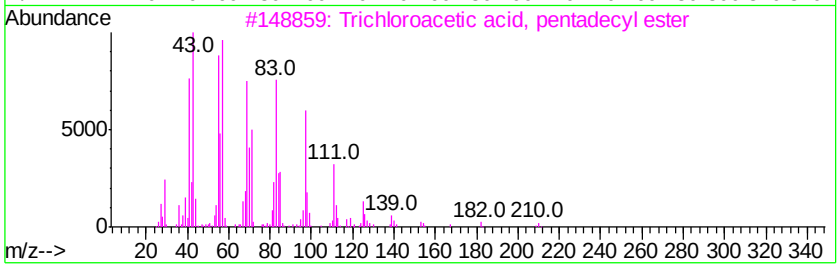
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	6.13 ng	313038	Chrysene-d12	13.72

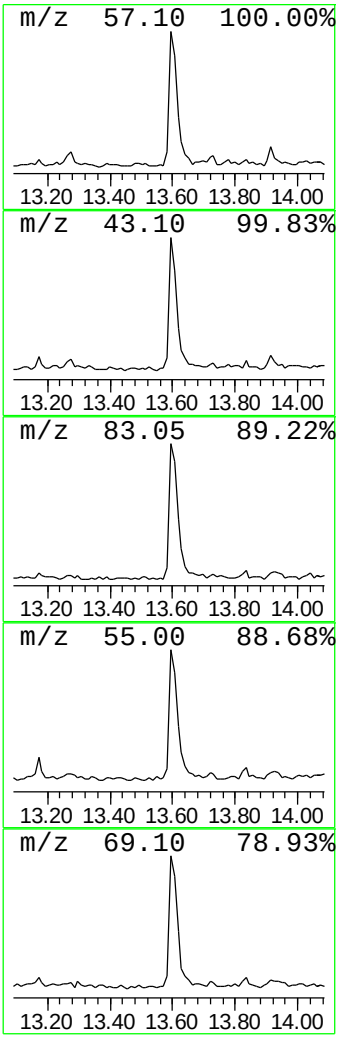
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	1-Tetracosanol	354	C24H50O	000506-51-4	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	11-Tricosene	322	C23H46	052078-56-5	86
5	1-Docosene	308	C22H44	001599-67-3	81











Tentatively Identified Compound (LSC) summary

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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...	4.72	56.3	ng	3183480	1	6.59	1130630	20.0
unknown6.36	6.36	111.1	ng	6278830	1	6.59	1130630	20.0
Octadecane	10.54	2.5	ng	154225	4	11.10	1258550	20.0
n-Hexadecanoic acid	11.65	3.4	ng	213244	4	11.10	1258550	20.0
Trichloroacetic a...	13.59	6.1	ng	313038	5	13.72	1020790	20.0