LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101215\
Data File : BF082228.D
Acq On : 12 Oct 2015 19:12
Operator : UM/IZ
Sample : G3990-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-PMW-9D

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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-BF101015.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	4.994	248	250	257	rBV	280683	335945	14.14%	2.237%
2	5.417	285	287	290	rBV	683403	678295	28.55%	4.516%
3	6.457	376	378	381	rBV2	328712	415266	17.48%	2.765%
4	6.594	388	390	393	rBV	1381882	1318684	55.50%	8.779%
5	6.834	409	411	413	rBV	277049	325482	13.70%	2.167%
6	6.983	422	424	427	rBV	1288356	1299398	54.68%	8.651%
7	7.406	458	461	463	rBV	847115	1071543	45.10%	7.134%
8	8.114	521	523	526	rBV	419686	451415	19.00%	3.005%
9	9.200	615	618	620	rBV	2411732	2331518	98.12%	15.522%
10	9.589	650	652	654	rBV	113610	110285	4.64%	0.734%
11	9.875	674	677	679	rBV	655228	583787	24.57%	3.886%
12	10.298	709	714	716	rBV2	28907	39911	1.68%	0.266%
13	10.618	739	742	743	rVB	21171	28264	1.19%	0.188%
14	10.663	743	746	749	rBV	1335408	1428508	60.12%	9.510%
15	10.778	754	756	758	rVB	26988	34410	1.45%	0.229%
16	11.223	793	795	796	rBV	46574	41274	1.74%	0.275%
17	11.360	805	807	809	rBV	679053	607682	25.57%	4.046%
18	11.886	851	853	857	rBV2	81095	108827	4.58%	0.724%
19	12.675	920	922	925	rBV	30131	37684	1.59%	0.251%
20	12.949	943	946	949	rBV	2401391	2376188	100.00%	15.819%
21	13.509	992	995	997	rBV2	26607	40063	1.69%	0.267%
22	13.841	1022	1024	1031	rVB	74438	103537	4.36%	0.689%
23	14.001	1035	1038	1045	rVB	677501	681246	28.67%	4.535%
24	15.441	1161	1164	1177	rVB	316758	522596	21.99%	3.479%
25	16.104	1219	1222	1227	rVB3	28697	49173	2.07%	0.327%

Sum of corrected areas: 15020981

LSC Report - Integrated Chromatogram

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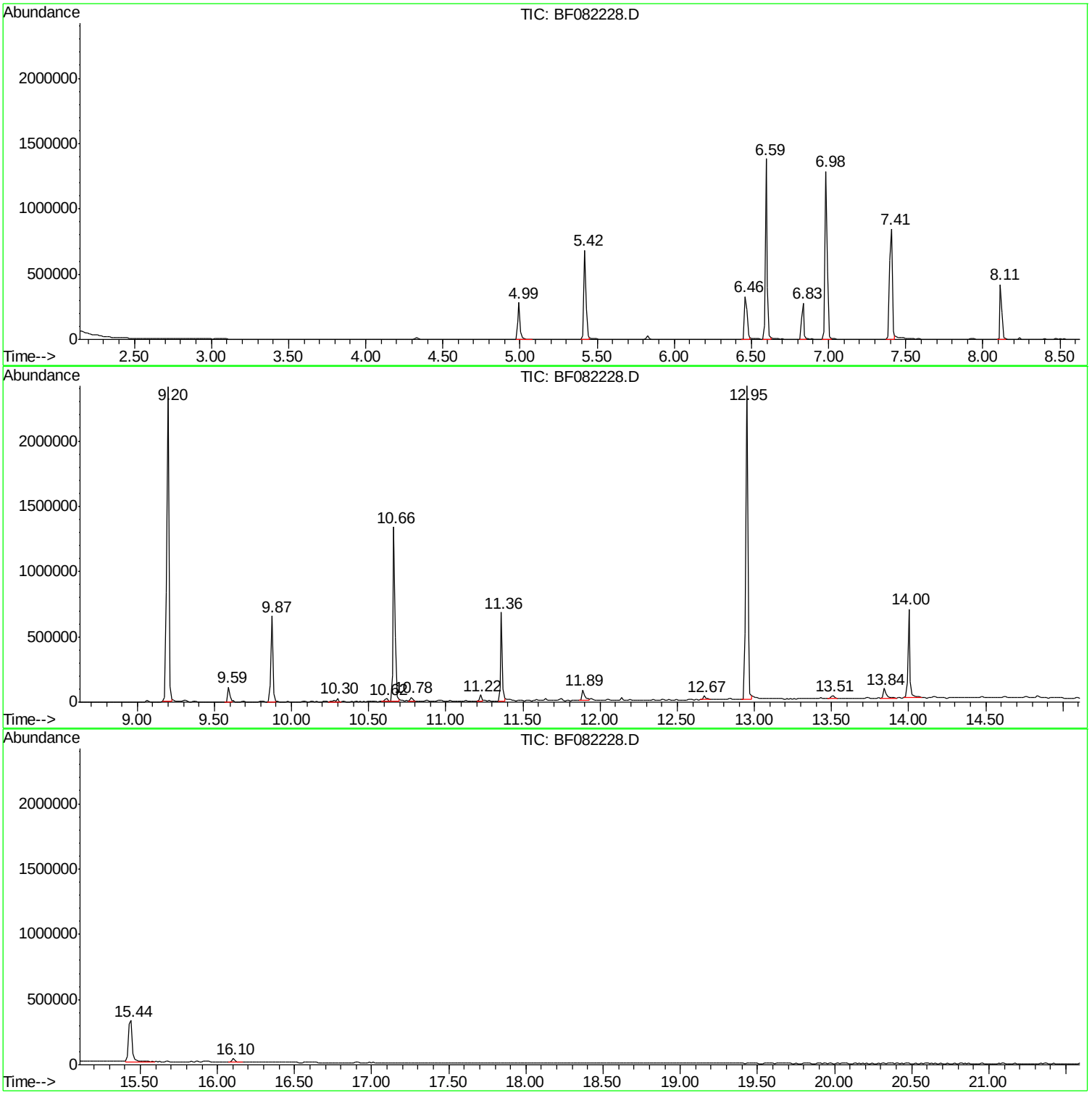
Instrument : BNA_F
ClientSampleId : TE-PMW-9D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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Operator : UM/IZ
Sample : G3990-08
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Instrument : BNA_F
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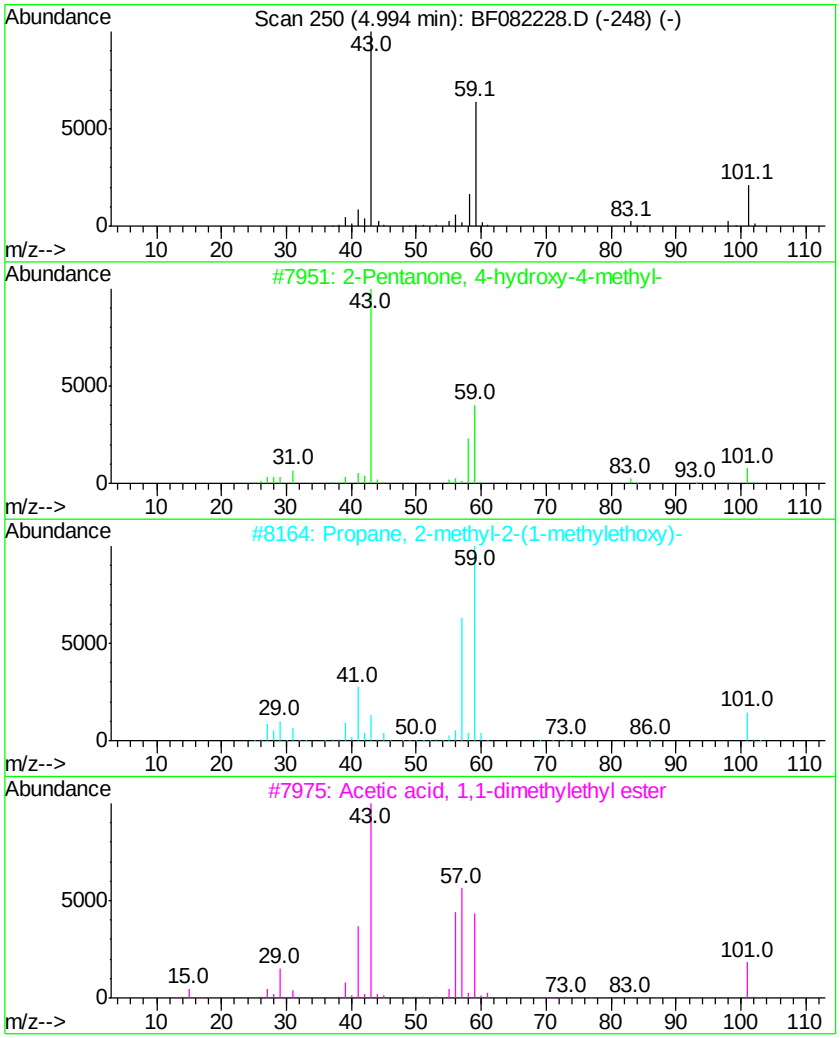
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

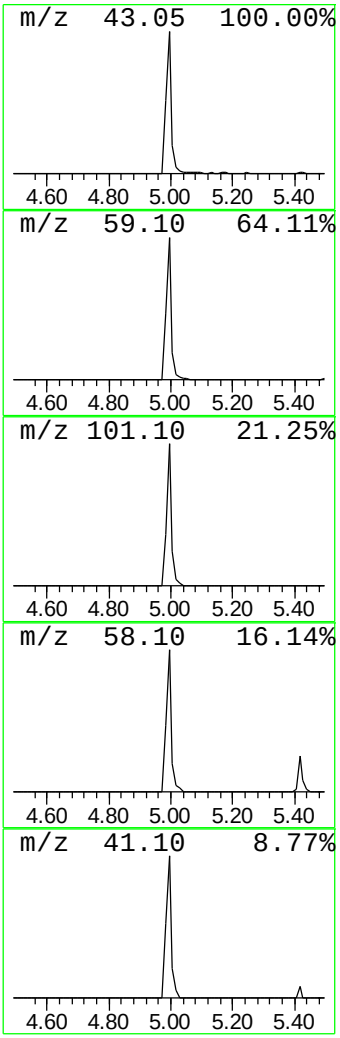
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	20.64 ng	335945	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Sample : G3990-08
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Instrument : BNA_F
ClientSampleId : TE-PMW-9D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Integration Parameters: LSCINT.P

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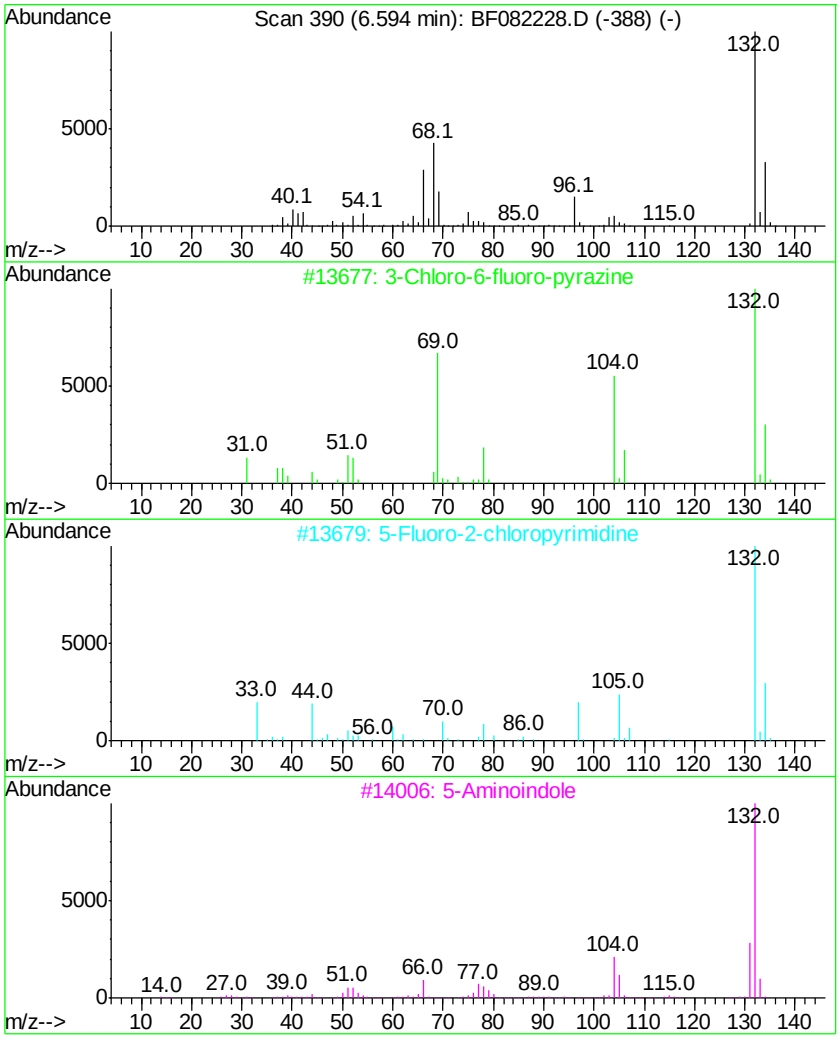
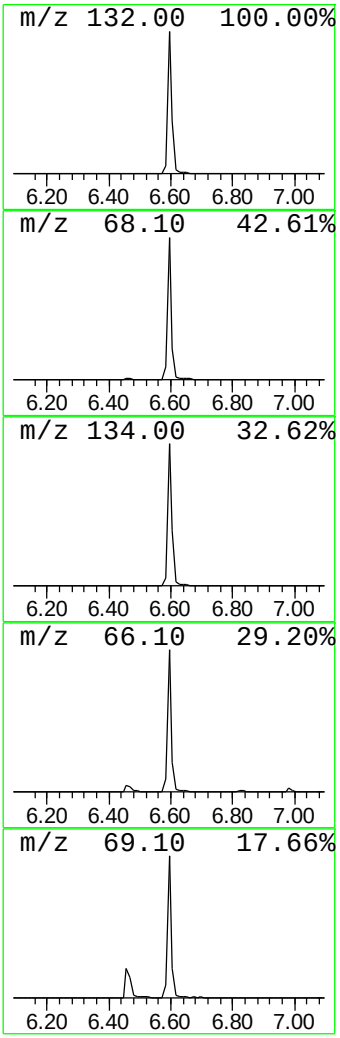
Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	81.03 ng	1318680	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Data File : BF082228.D
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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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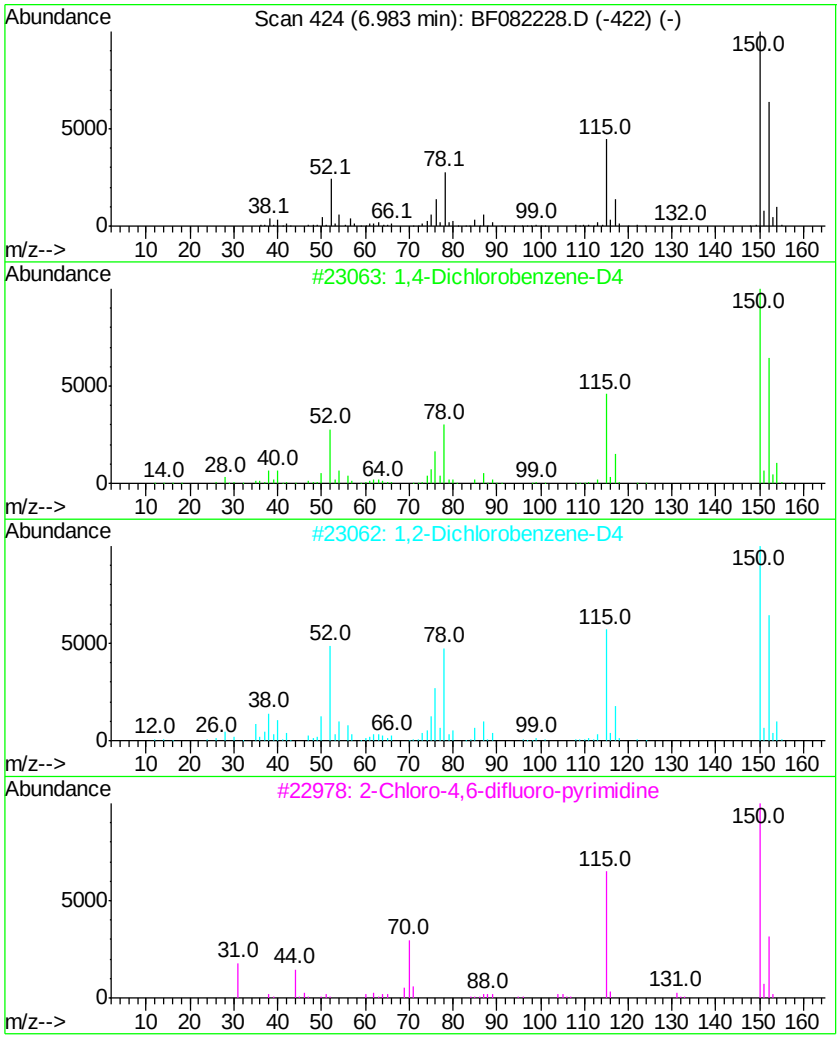
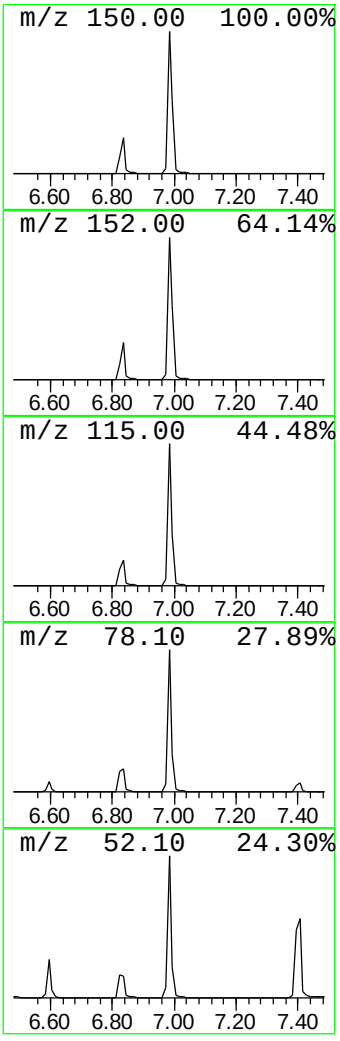
Peak Number 3 1,4-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	79.84 ng	1299400	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	94
2	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	91
3	2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	38
4	2-Bromo-3'-nitroacetophenone	243	C8H6BrNO3	002227-64-7	14
5	2-Bromo-2'-nitroacetophenone	243	C8H6BrNO3	006851-99-6	12





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Instrument : BNA_F
ClientSampleId : TE-PMW-9D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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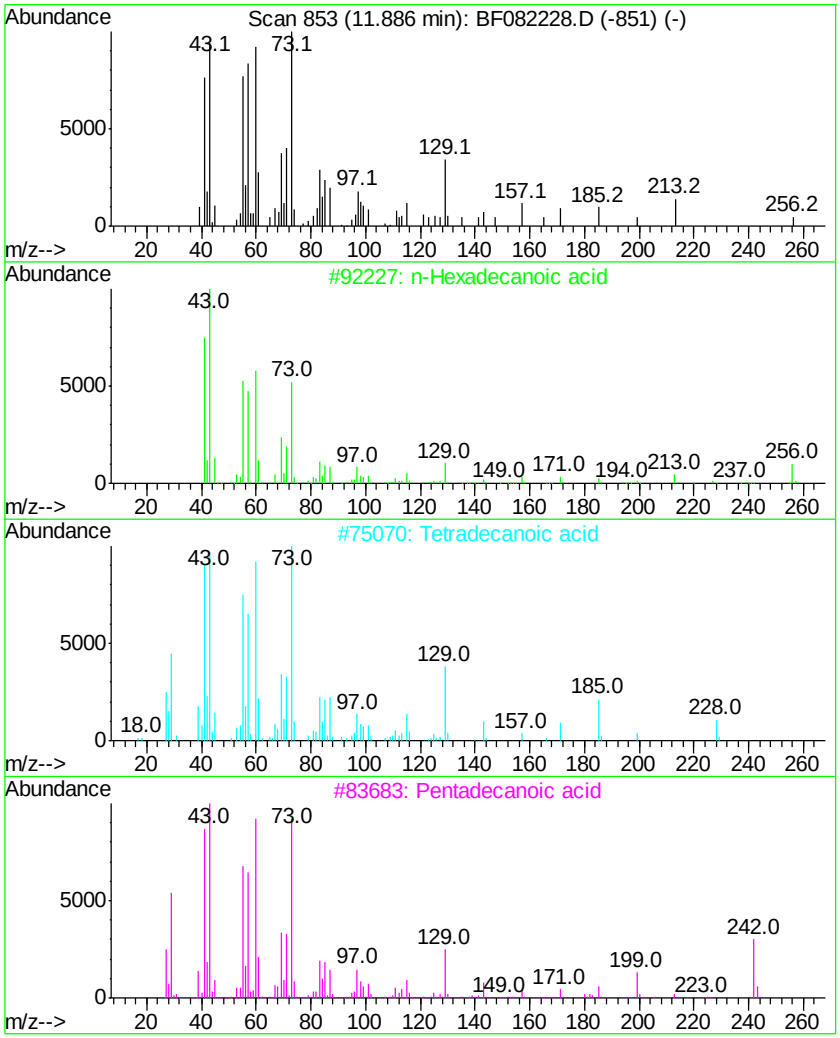
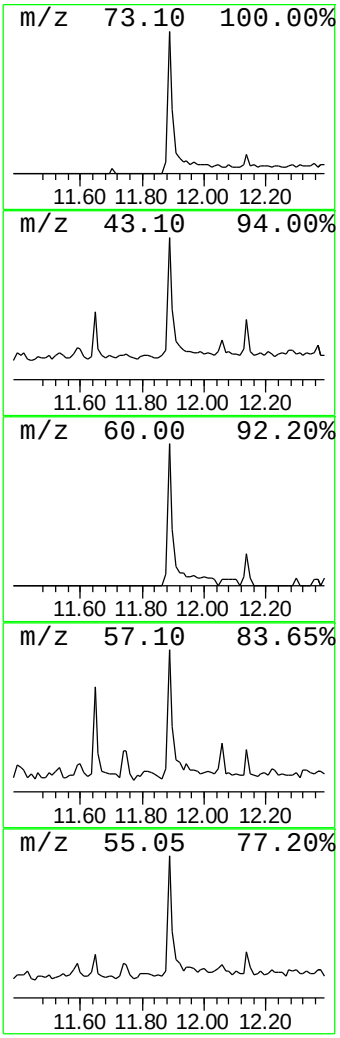
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	3.58 ng	108827	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	50





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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TE-PMW-9D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

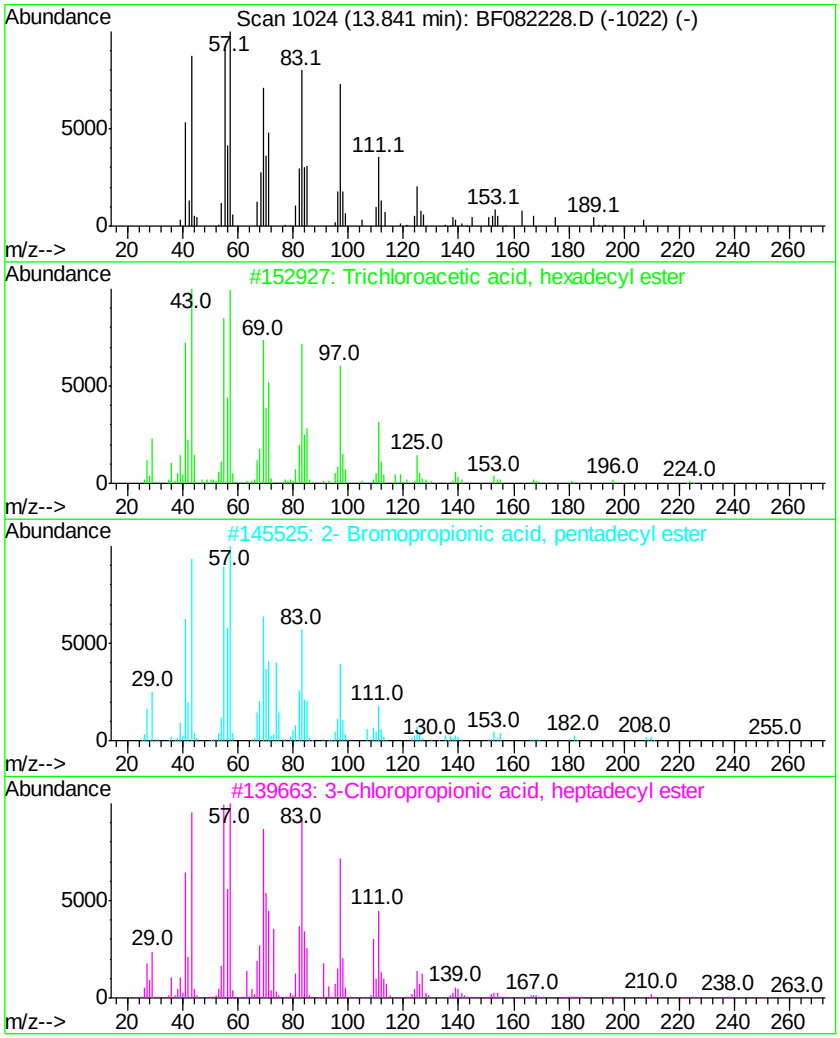
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

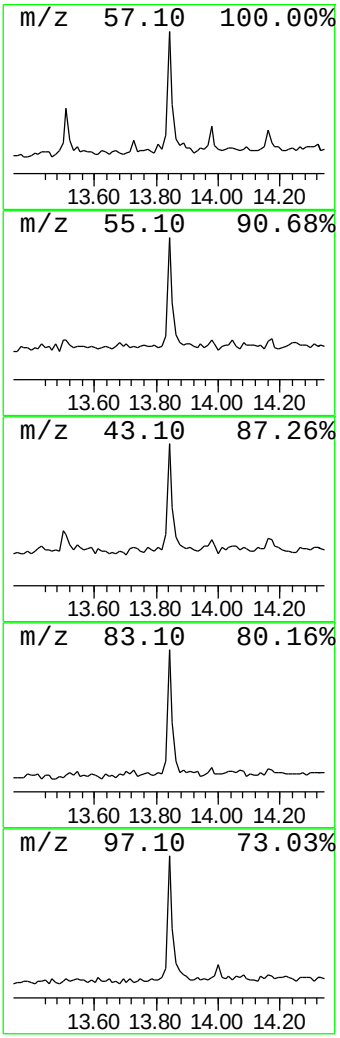
****

Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.04 ng	103537	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	87





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...	4.99	20.6	ng	335945	1	6.83	325482	20.0
3-Chloro-6-fluoro...	6.59	81.0	ng	1318680	1	6.83	325482	20.0
1,4-Dichlorobenze...	6.98	79.8	ng	1299400	1	6.83	325482	20.0
n-Hexadecanoic acid	11.89	3.6	ng	108827	4	11.36	607682	20.0
Trichloroacetic a...	13.84	3.0	ng	103537	5	14.00	681246	20.0