LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122215\
Data File : BF084023.D
Acq On : 23 Dec 2015 7:32
Operator : UM/SJ
Sample : G4920-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-012

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-BF122215.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	5.013	254	256	264	rBB	164418	228676	16.87%	1.908%
2	5.447	292	294	297	rBV	1215798	1111194	81.95%	9.270%
3	6.476	382	384	386	rBV	1134653	1091258	80.48%	9.104%
4	6.602	393	395	397	rBV	1421431	1271712	93.79%	10.609%
5	6.830	413	415	417	rBV	271811	256823	18.94%	2.142%
6	6.979	426	428	431	rBV	737441	935435	68.99%	7.804%
7	7.390	462	464	467	rBV	766585	722200	53.26%	6.025%
8	8.110	525	527	530	rBV	403992	350606	25.86%	2.925%
9	9.196	619	622	624	rBV	943655	1355890	100.00%	11.311%
10	9.585	654	656	658	rBV	251618	206811	15.25%	1.725%
11	9.870	678	681	683	rBB	372411	412171	30.40%	3.438%
12	10.305	717	719	721	rVB	22183	18727	1.38%	0.156%
13	10.659	747	750	752	rBV	950722	1005667	74.17%	8.390%
14	10.773	758	760	765	rBV	22213	30457	2.25%	0.254%
15	11.219	798	799	801	rBV	11732	15553	1.15%	0.130%
16	11.356	809	811	813	rBV	334115	431717	31.84%	3.601%
17	12.762	932	934	936	rBB	92403	73784	5.44%	0.616%
18	12.842	936	941	942	rBB2	13334	22285	1.64%	0.186%
19	12.934	947	949	952	rBV	1353119	1257067	92.71%	10.487%
20	13.459	993	995	997	rBV	43588	56389	4.16%	0.470%
21	13.517	997	1000	1004	rVB2	9213	21323	1.57%	0.178%
22	13.837	1025	1028	1036	rBV	88059	141551	10.44%	1.181%
23	13.985	1039	1041	1044	rVB	434741	437085	32.24%	3.646%
24	14.157	1054	1056	1058	rBV	24974	26854	1.98%	0.224%
25	14.454	1080	1082	1087	rBV2	16536	28094	2.07%	0.234%
26	14.751	1106	1108	1110	rBV	13410	16620	1.23%	0.139%
27	15.071	1135	1136	1139	rBV	10702	15245	1.12%	0.127%
28	15.414	1164	1166	1175	rVB	219869	342845	25.29%	2.860%
29	15.848	1202	1204	1206	rBV	9519	15257	1.13%	0.127%
30	15.905	1206	1209	1218	rVB3	5671	18742	1.38%	0.156%
31	16.328	1241	1246	1249	rBV2	8054	18670	1.38%	0.156%
32	16.877	1291	1294	1300	rBV4	6163	16772	1.24%	0.140%
33	17.540	1345	1352	1356	rVB3	5526	16580	1.22%	0.138%
34	19.243	1496	1501	1509	rVB6	3604	17136	1.26%	0.143%

LSC Area Percent Report

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Data File : BF084023.D
Acq On : 23 Dec 2015 7:32
Operator : UM/SJ
Sample : G4920-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IM-CLAY-012

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-BF122215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

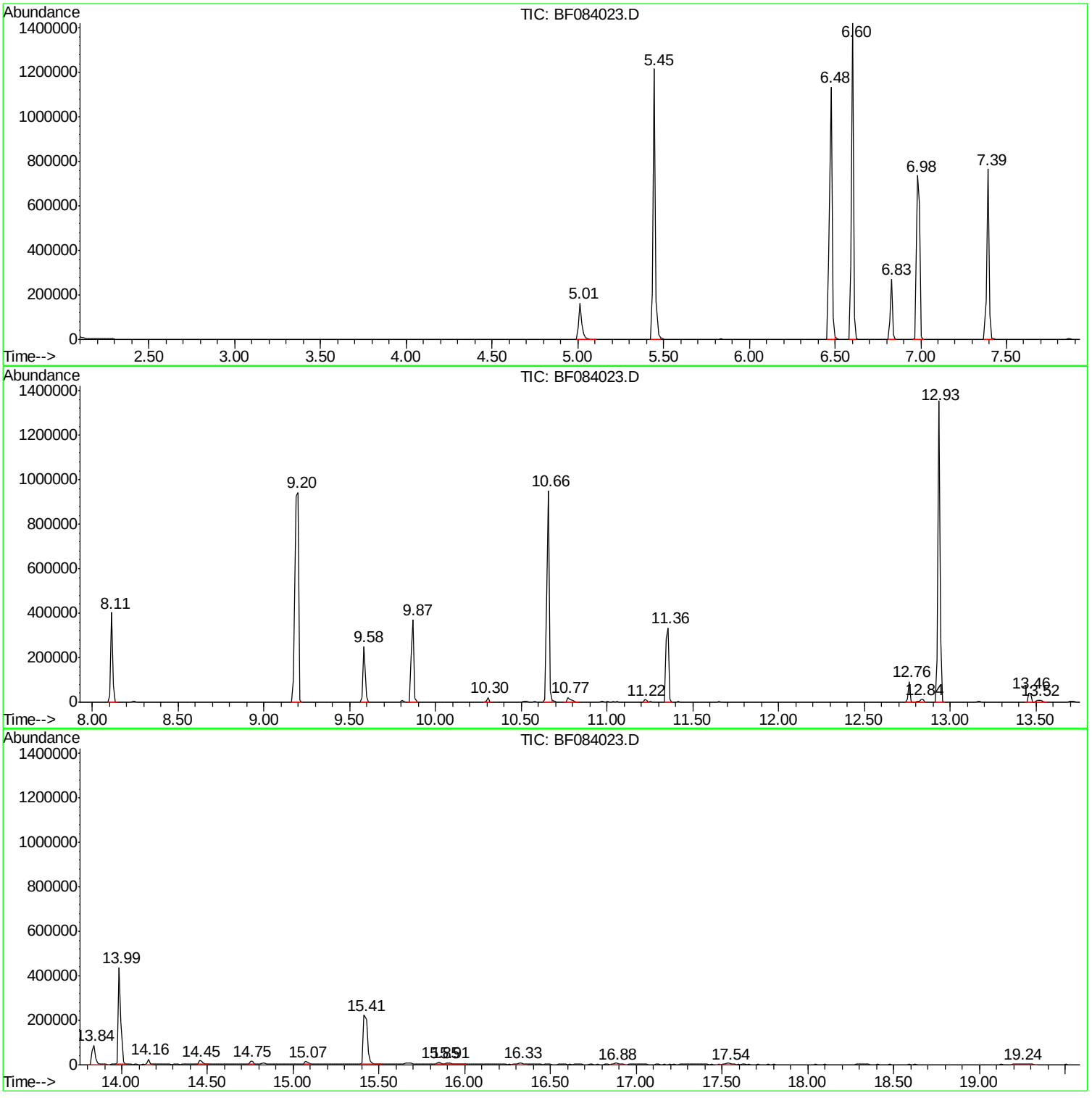
Sum of corrected areas: 11987196

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122215\
Data File : BF084023.D
Acq On : 23 Dec 2015 7:32
Operator : UM/SJ
Sample : G4920-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IM-CLAY-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122215.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\BF122215\
Data File : BF084023.D
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Operator : UM/SJ
Sample : G4920-07
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Instrument : BNA_F
ClientSampleId : IM-CLAY-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

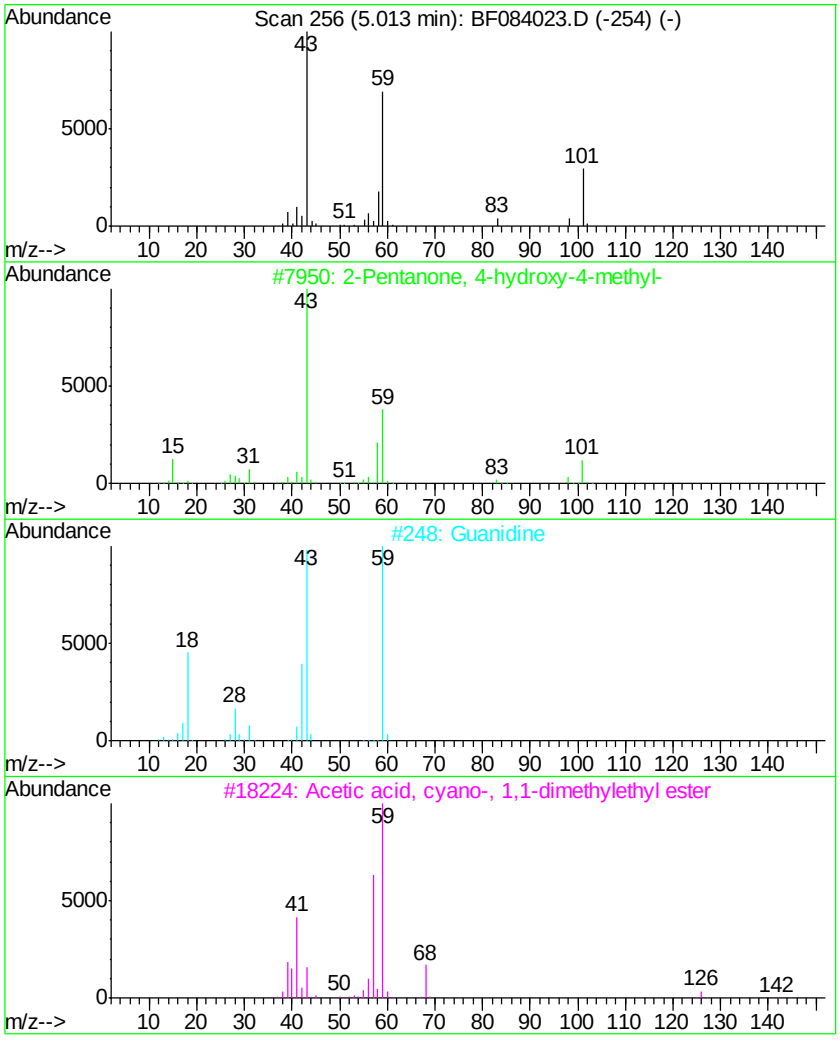
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

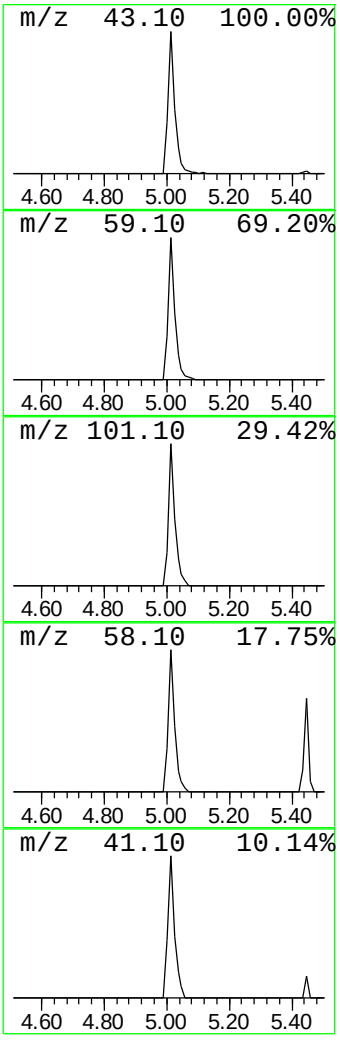
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	17.81 ng	228676	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	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5	Acetone	58	C3H6O	000067-64-1	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122215\
Data File : BF084023.D
Acq On : 23 Dec 2015 7:32
Operator : UM/SJ
Sample : G4920-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

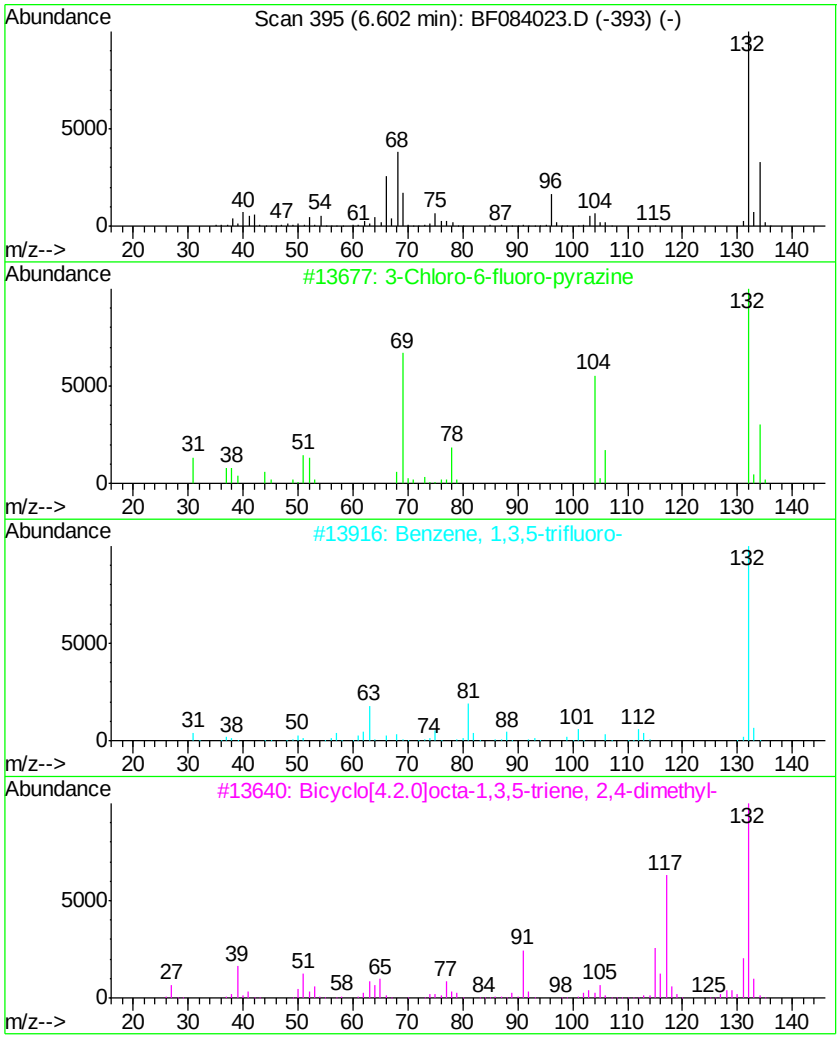
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

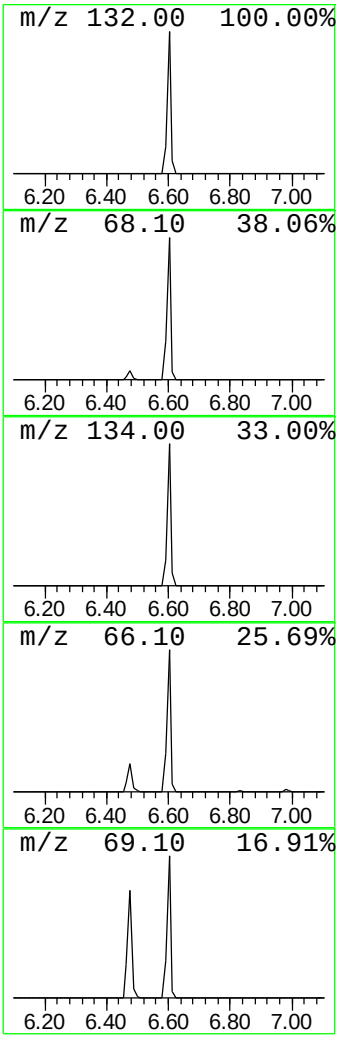
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	99.03 ng	1271710	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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122215\
Data File : BF084023.D
Acq On : 23 Dec 2015 7:32
Operator : UM/SJ
Sample : G4920-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122215.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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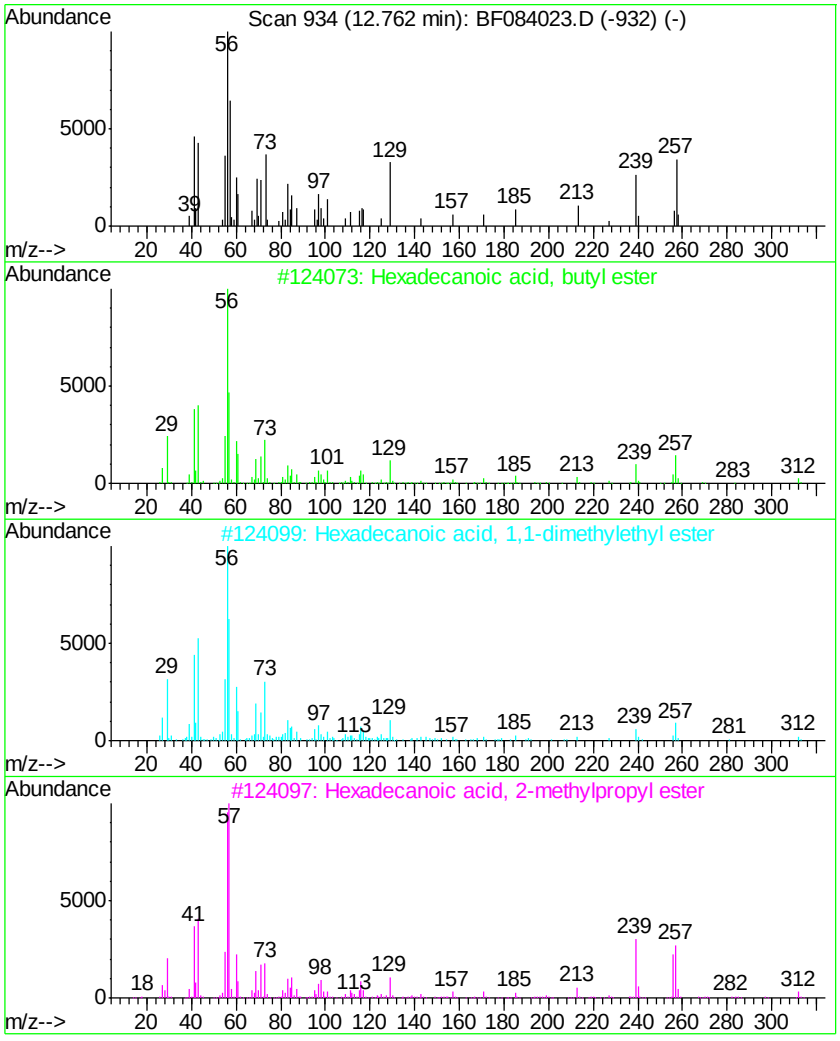
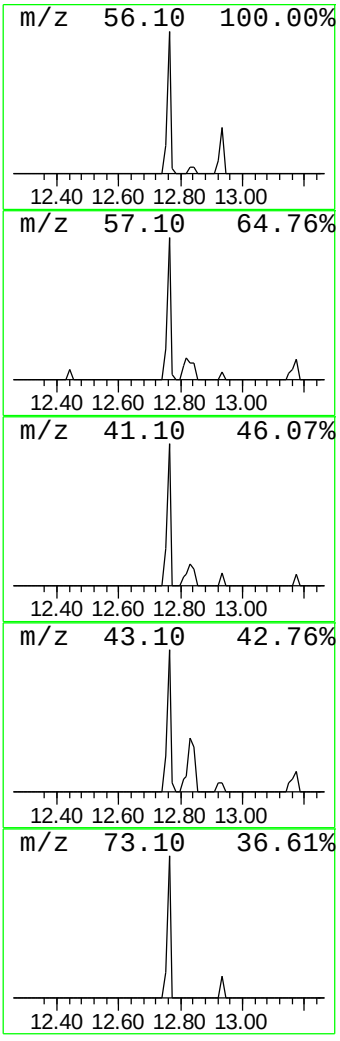
Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	3.38 ng	73784	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	59
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	47
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	45
4	Nipecotic acid	129	C6H11NO2	000498-95-3	37
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	22





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Sample : G4920-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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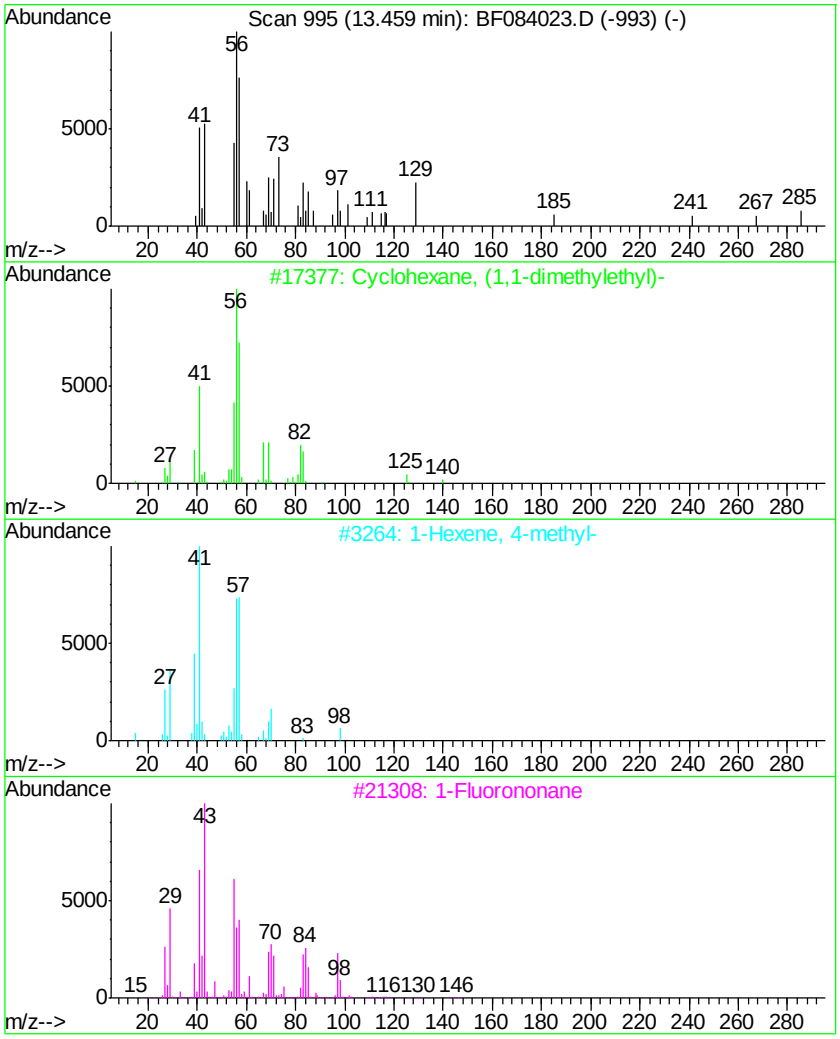
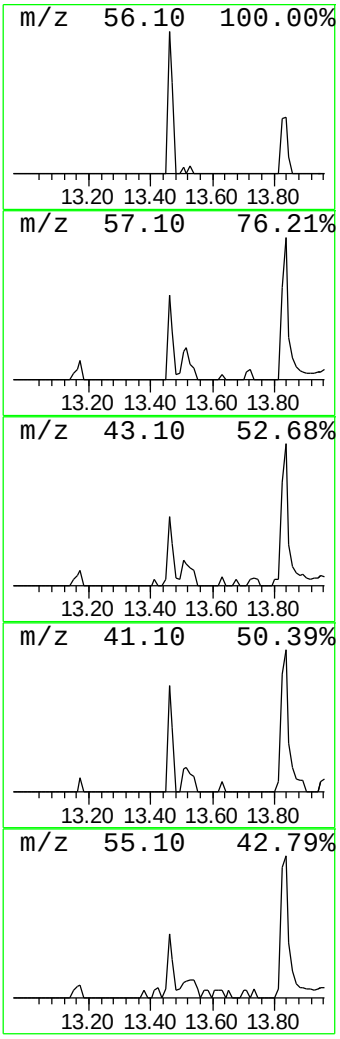
****

Peak Number 5 unknown13.46 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	2.58 ng	56389	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	25
2	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	22
3	1-Fluorononane	146	C9H19F	000463-18-3	16
4	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	14
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	14





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122215\
Data File : BF084023.D
Acq On : 23 Dec 2015 7:32
Operator : UM/SJ
Sample : G4920-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-012

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

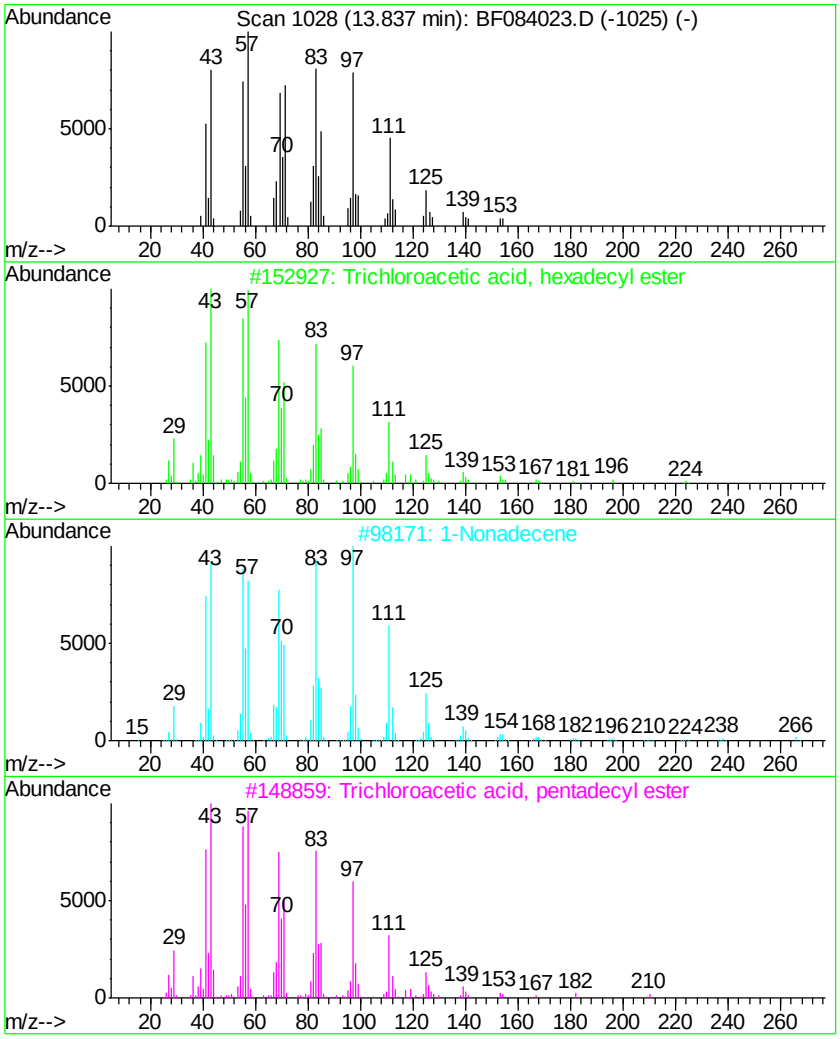
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

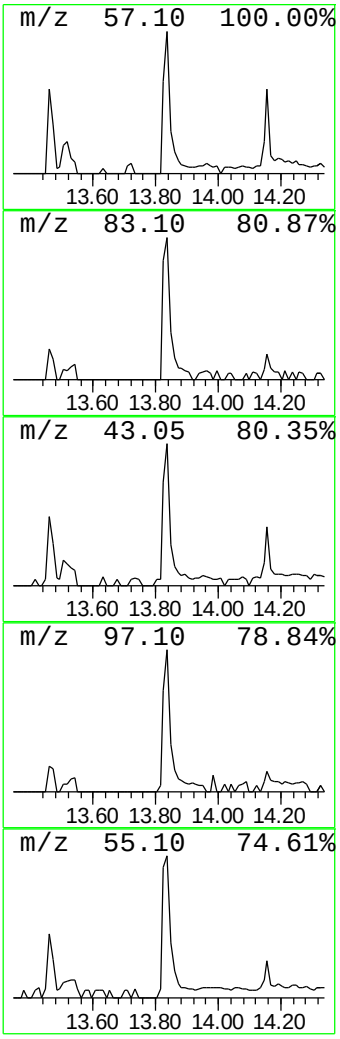
****

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	6.48 ng	141551	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	1-Nonadecene	266	C19H38	018435-45-5	81
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74
4	1-Docosene	308	C22H44	001599-67-3	74
5	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	74





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
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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...	5.01	17.8	ng	228676	1	6.83	256823	20.0
unknown6.60	6.60	99.0	ng	1271710	1	6.83	256823	20.0
Hexadecanoic acid...	12.76	3.4	ng	73784	5	13.99	437085	20.0
unknown13.46	13.46	2.6	ng	56389	5	13.99	437085	20.0
Trichloroacetic a...	13.84	6.5	ng	141551	5	13.99	437085	20.0