LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122215\
Data File : BF084021.D
Acq On : 23 Dec 2015 6:36
Operator : UM/SJ
Sample : G4920-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-008

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	265	rBB	180893	262079	11.38%	1.715%
2	5.447	292	294	297	rBV	1206286	1176874	51.11%	7.699%
3	6.476	382	384	387	rBV	1079935	1152611	50.06%	7.540%
4	6.602	393	395	398	rBV	1486228	1325614	57.57%	8.672%
5	6.830	413	415	417	rBV	280822	242655	10.54%	1.587%
6	6.990	426	429	431	rBV	1402235	1789283	77.71%	11.705%
7	7.390	462	464	467	rBV	1324182	1327881	57.67%	8.687%
8	8.110	525	527	530	rBV	659130	579061	25.15%	3.788%
9	9.196	619	622	624	rBV	1683025	2302610	100.00%	15.064%
10	9.585	654	656	658	rBV	556844	456273	19.82%	2.985%
11	9.802	673	675	678	rBV	26421	28370	1.23%	0.186%
12	9.870	678	681	683	rVV	596647	633482	27.51%	4.144%
13	10.305	717	719	721	rVB	40689	32836	1.43%	0.215%
14	10.659	747	750	752	rBV	1019058	1069515	46.45%	6.997%
15	10.773	758	760	764	rBV	42122	50611	2.20%	0.331%
16	11.219	798	799	801	rBV	18402	24463	1.06%	0.160%
17	11.356	809	811	813	rBV	288287	399675	17.36%	2.615%
18	12.762	931	934	936	rBV	66628	53086	2.31%	0.347%
19	12.934	947	949	952	rBV	1361537	1377344	59.82%	9.011%
20	13.459	994	995	997	rBB	34219	40721	1.77%	0.266%
21	13.837	1025	1028	1034	rBV	116155	200462	8.71%	1.311%
22	13.985	1039	1041	1044	rVB	362558	386512	16.79%	2.529%
23	14.157	1053	1056	1062	rBV	23909	24010	1.04%	0.157%
24	14.465	1080	1083	1087	rBV	19794	32661	1.42%	0.214%
25	15.414	1164	1166	1175	rVB	187868	293122	12.73%	1.918%
26	15.905	1206	1209	1213	rBV	10297	24164	1.05%	0.158%

Sum of corrected areas: 15285975

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Misc :
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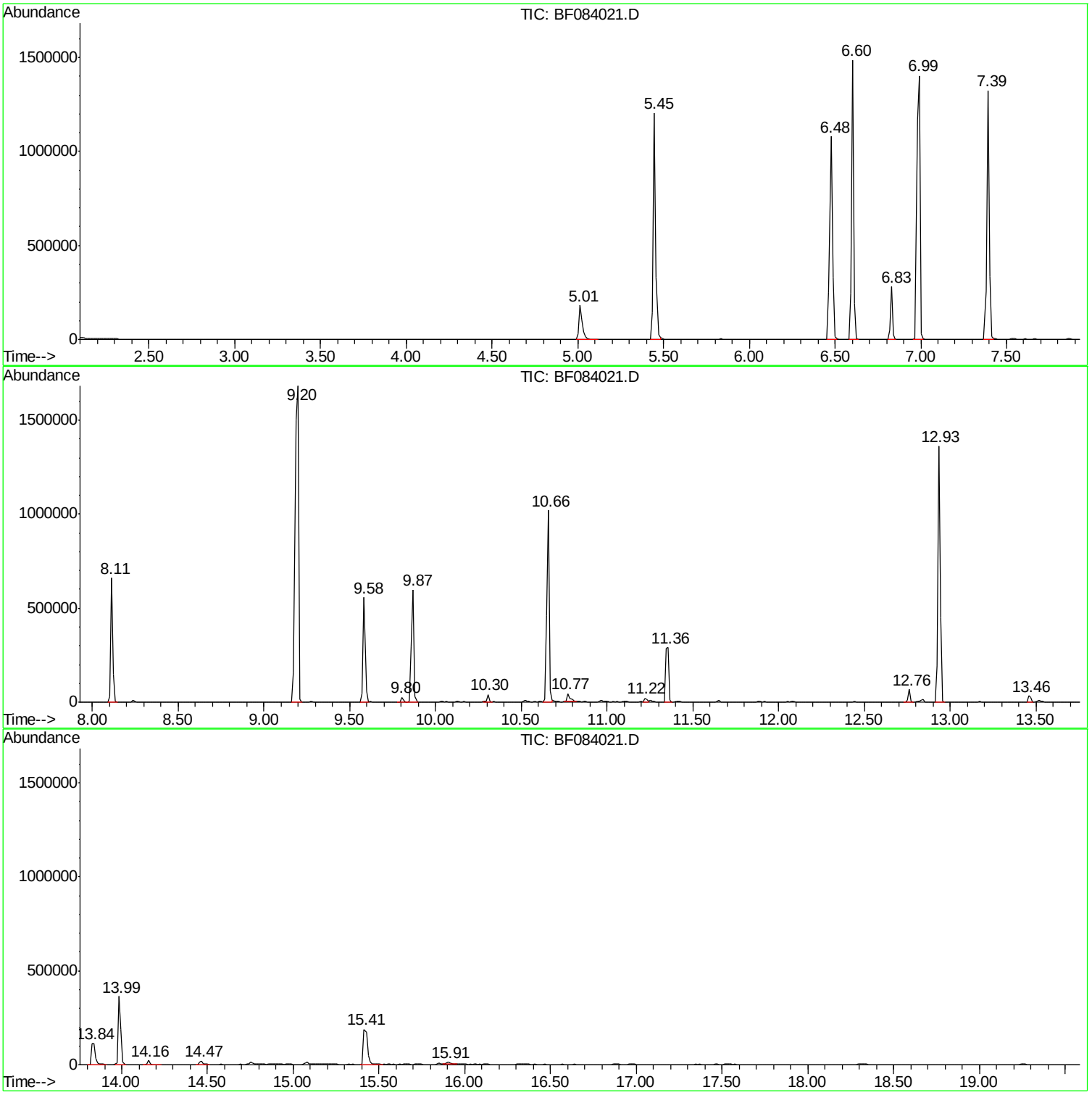
Instrument :
BNA_F
ClientSampleId :
IM-CLAY-008

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 : BF084021.D
Acq On : 23 Dec 2015 6:36
Operator : UM/SJ
Sample : G4920-03
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Instrument : BNA_F
ClientSampleId : IM-CLAY-008

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

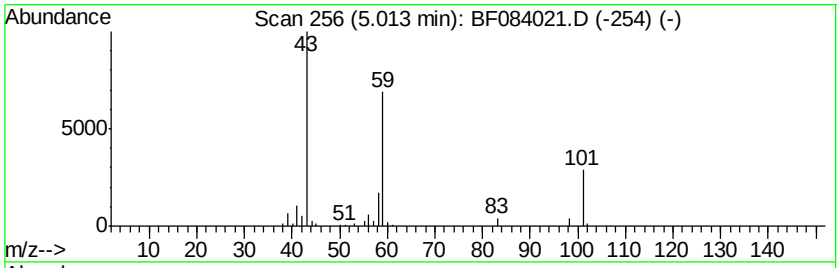
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

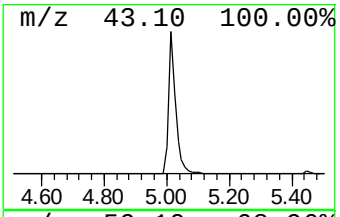
****

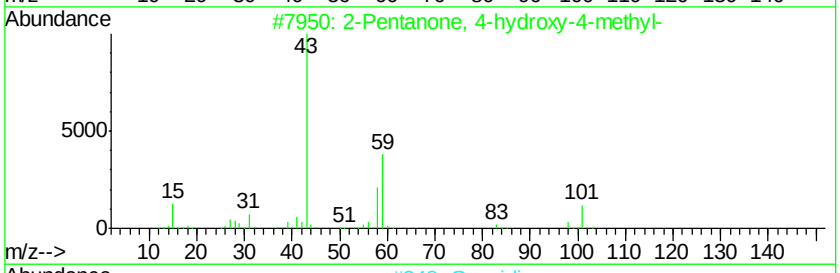
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

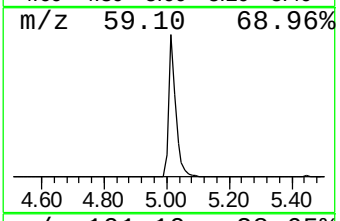
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	21.60 ng	262079	1,4-Dichlorobenzene-d4	6.83

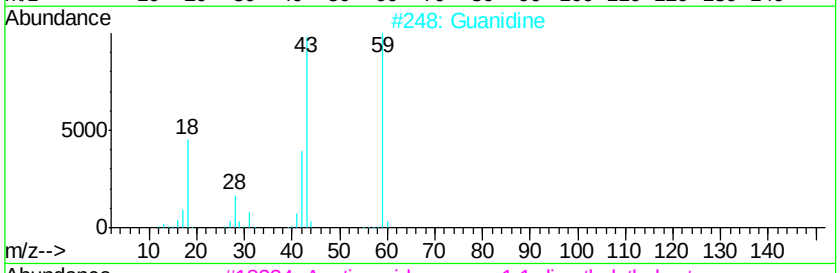
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2-Nonanone	142	C9H18O	000821-55-6	12
5	Acetone	58	C3H6O	000067-64-1	10

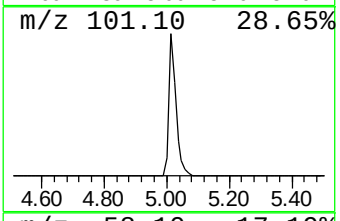


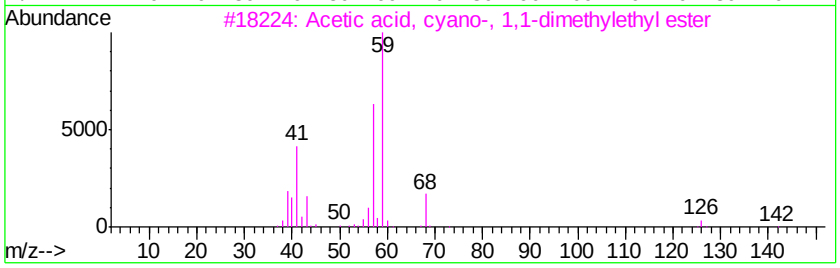


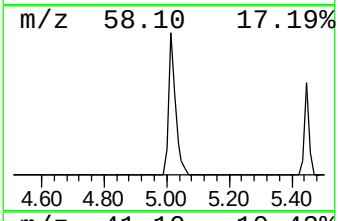


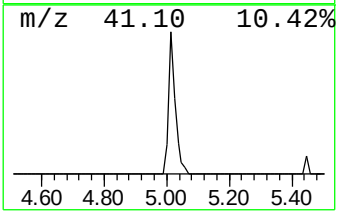












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Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-008

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

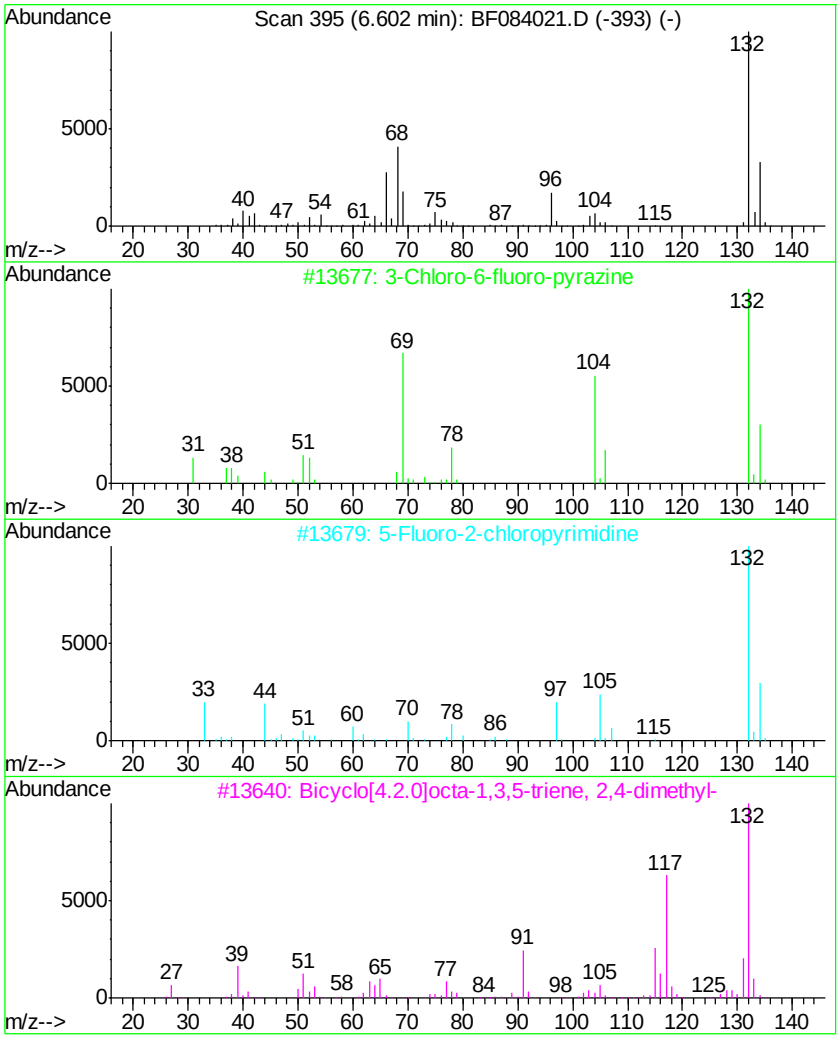
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

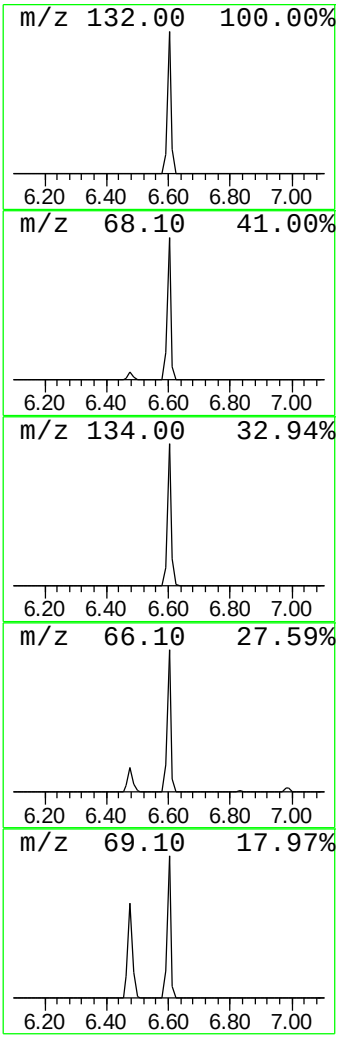
****

Peak Number 2 unknown6.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	109.26 ng	1325610	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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122215\
Data File : BF084021.D
Acq On : 23 Dec 2015 6:36
Operator : UM/SJ
Sample : G4920-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-008

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

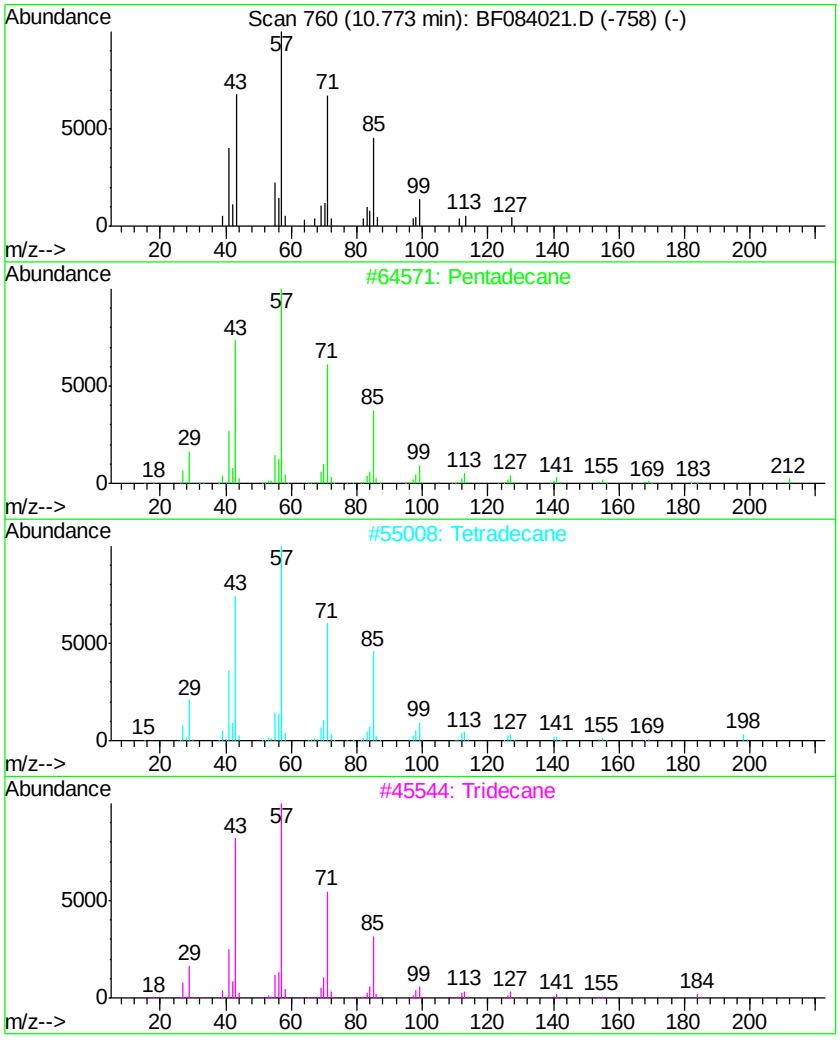
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

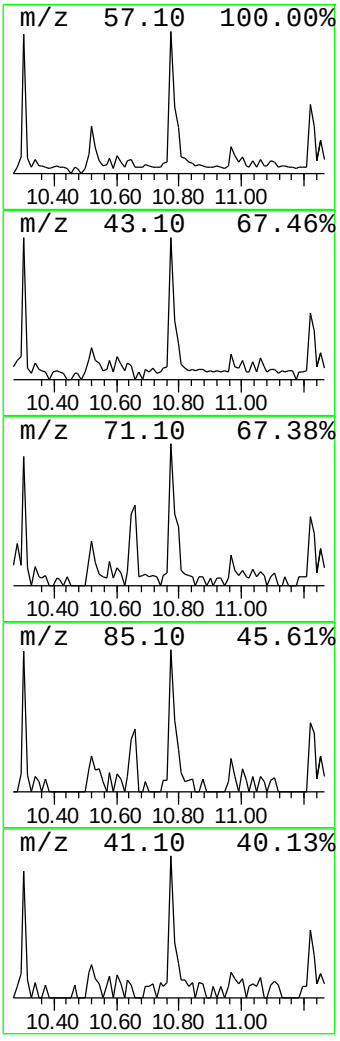
****

Peak Number 4 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.53 ng	50611	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Tridecane	184	C13H28	000629-50-5	78
4	Eicosane	282	C20H42	000112-95-8	78
5	Hexadecane	226	C16H34	000544-76-3	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122215\
Data File : BF084021.D
Acq On : 23 Dec 2015 6:36
Operator : UM/SJ
Sample : G4920-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-008

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

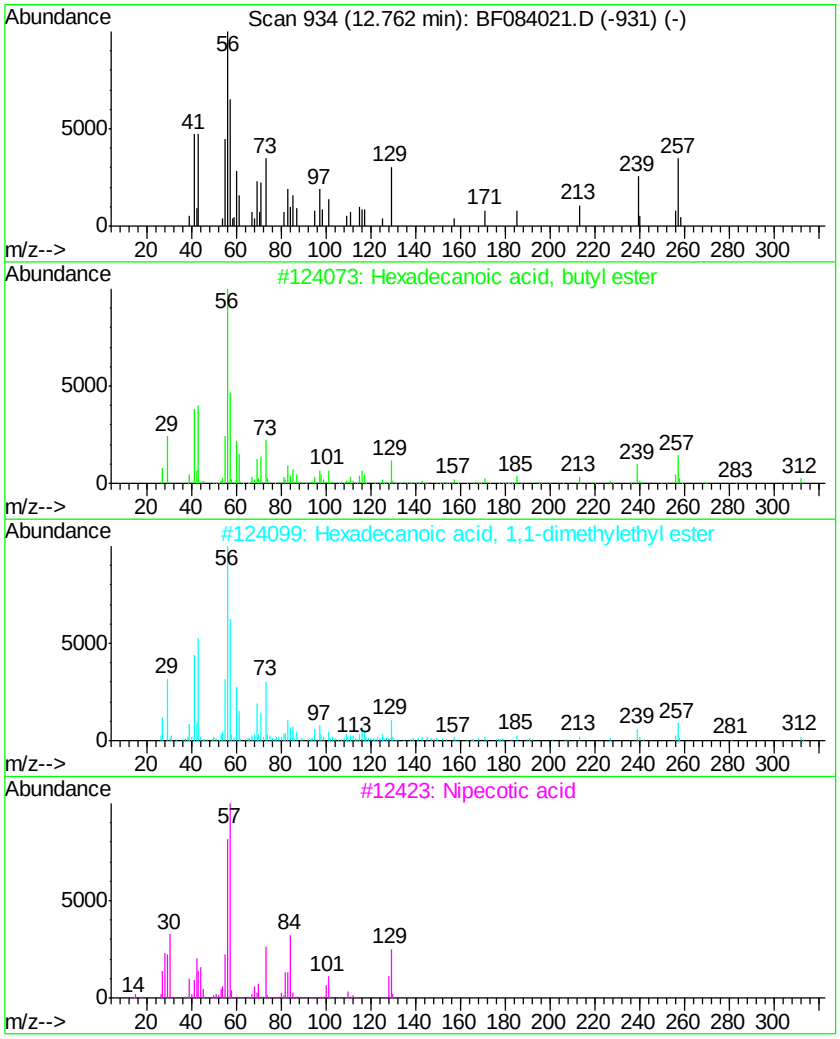
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

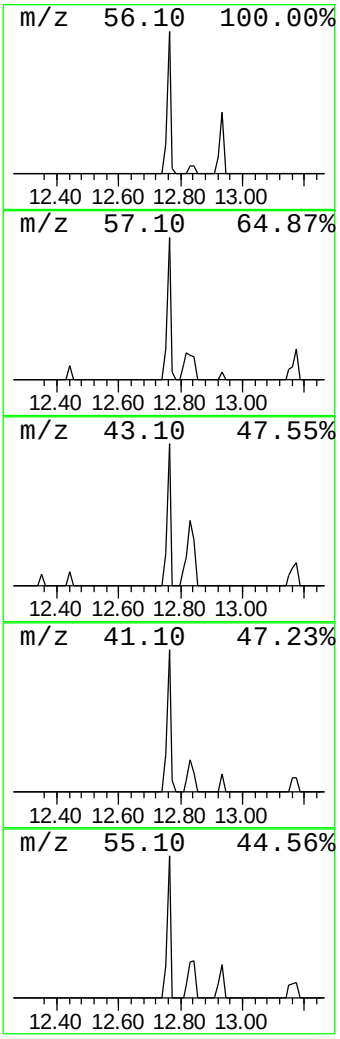
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	2.75 ng	53086	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3	Nipecotic acid	129	C6H11NO2	000498-95-3	38
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	22
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	22





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Sample : G4920-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-008

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

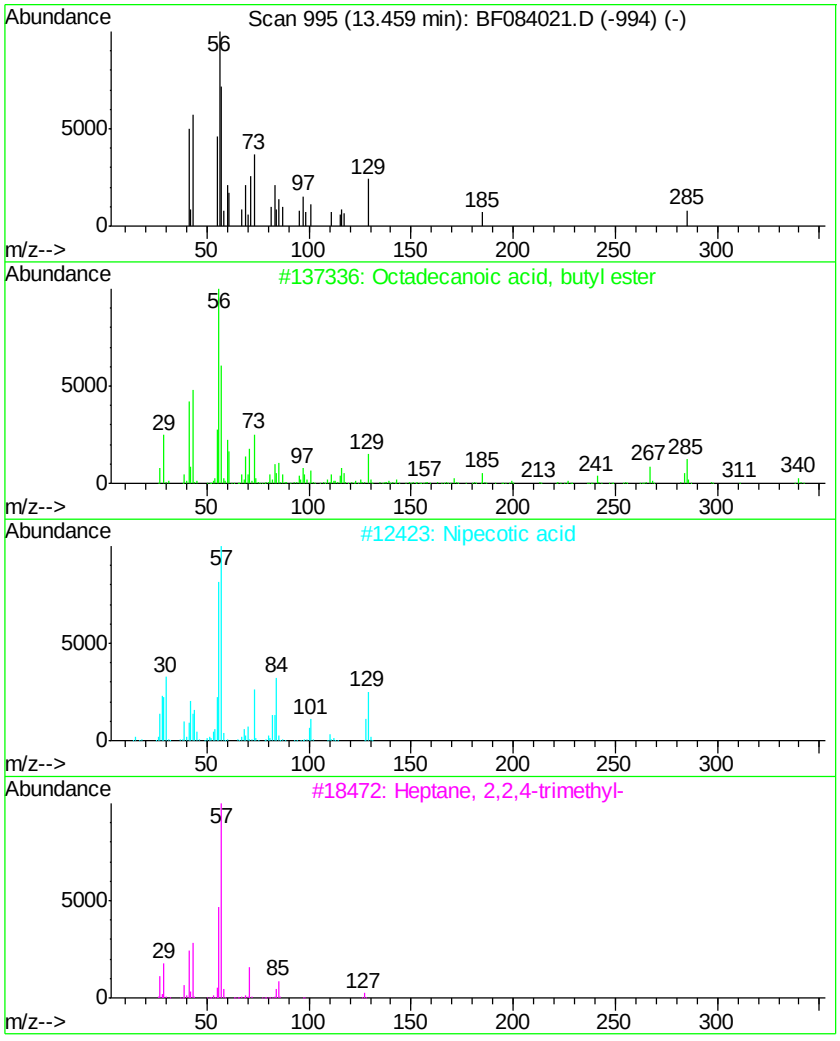
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

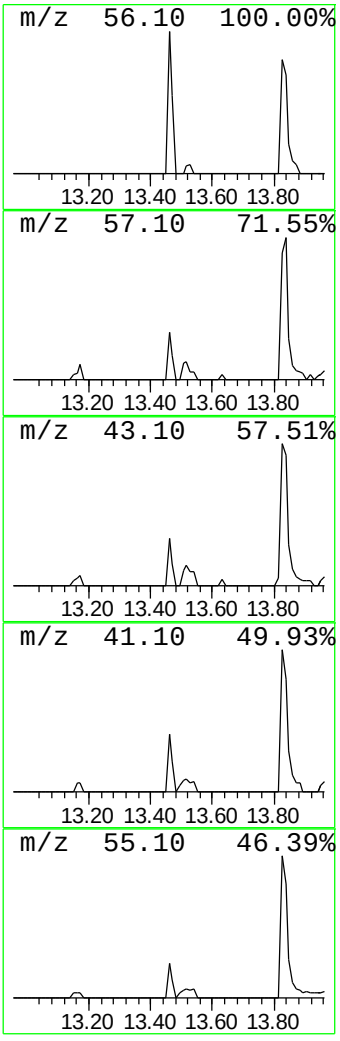
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	2.11 ng	40721	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	59
2	Nipecotic acid	129	C6H11NO2	000498-95-3	47
3	Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	32
4	2-Methyl-1-undecanol	186	C12H26O	010522-26-6	25
5	Chloromethyl 2-chloroundecanoate	268	C12H22Cl2O2	080418-88-8	25





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Sample : G4920-03
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-CLAY-008

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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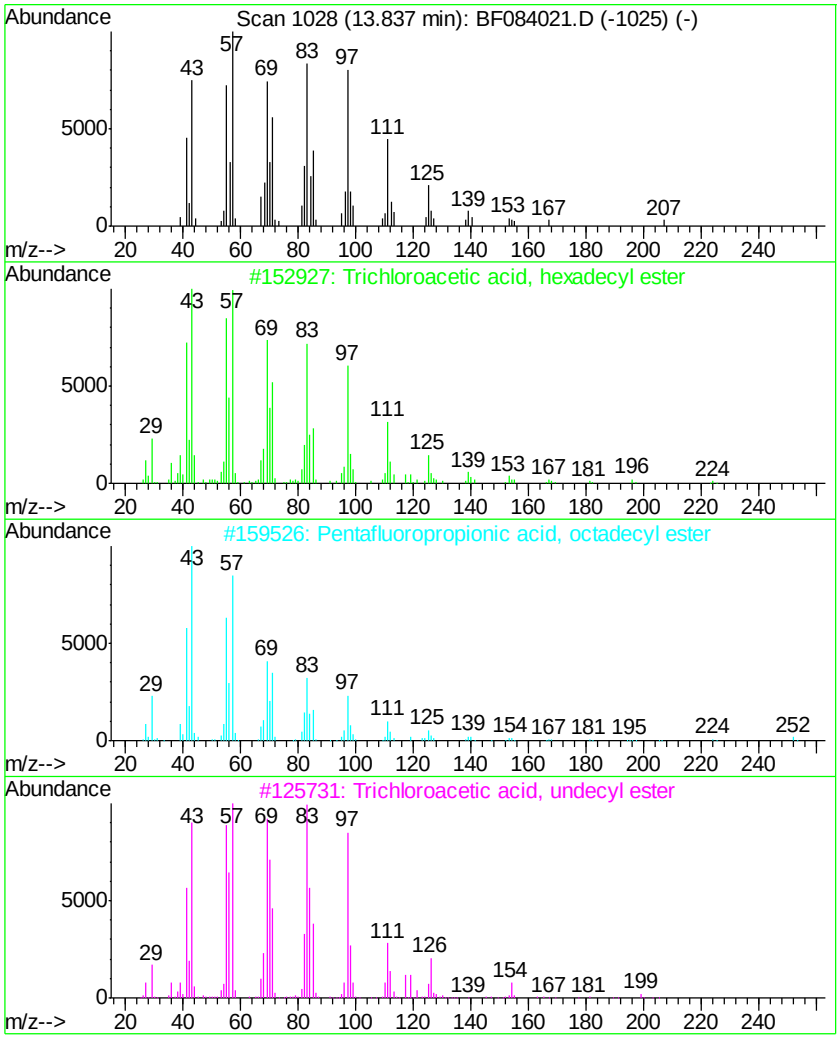
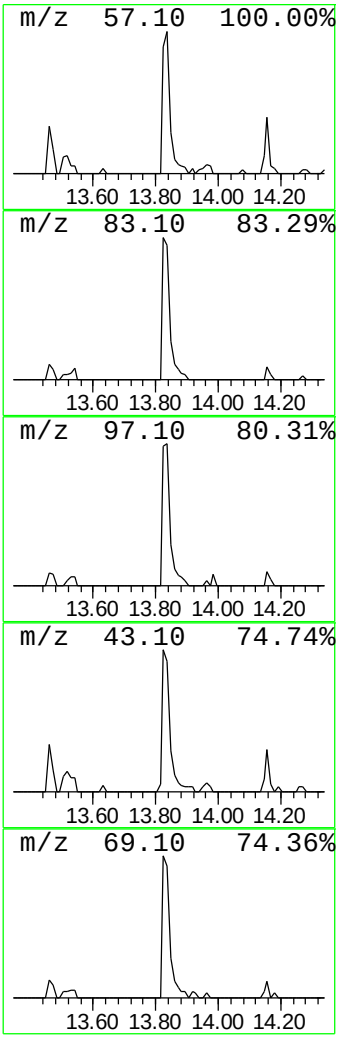
Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	10.37 ng	200462	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	83
3	Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	80
4	1-Docosene	308	C22H44	001599-67-3	76
5	17-Pentatriacontene	491	C35H70	006971-40-0	74





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	21.6	ng	262079	1	6.83	242655	20.0
unknown6.60	6.60	109.3	ng	1325610	1	6.83	242655	20.0
Pentadecane	10.77	2.5	ng	50611	4	11.36	399675	20.0
Hexadecanoic acid...	12.76	2.8	ng	53086	5	13.99	386512	20.0
Octadecanoic acid...	13.46	2.1	ng	40721	5	13.99	386512	20.0
Trichloroacetic a...	13.84	10.4	ng	200462	5	13.99	386512	20.0