LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
Data File : BF084300.D
Acq On : 6 Jan 2016 20:10
Operator : SJ/UM
Sample : H1017-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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-BF123115.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	5.047	256	259	264	rBV	610309	694607	8.61%	1.154%
2	5.127	264	266	268	rVB	83519	91598	1.14%	0.152%
3	5.470	294	296	299	rVB	3009712	3720641	46.11%	6.181%
4	6.510	384	387	389	rBV	2176838	2591766	32.12%	4.306%
5	6.636	395	398	401	rBV	6104138	5875926	72.82%	9.761%
6	6.865	416	418	420	rBV	2185375	1807391	22.40%	3.003%
7	7.025	429	432	434	rVB	6735983	5965777	73.93%	9.911%
8	7.276	451	454	460	rBV4	38881	95213	1.18%	0.158%
9	7.436	465	468	470	rBV	5281351	5485679	67.98%	9.113%
10	7.688	487	490	496	rVB2	52833	96236	1.19%	0.160%
11	8.156	528	531	533	rBV	2436089	2387993	29.59%	3.967%
12	8.522	557	563	565	rBV2	37980	110432	1.37%	0.183%
13	8.568	565	567	571	rVB4	55807	121477	1.51%	0.202%
14	9.231	622	625	628	rBV	7652145	8069306	100.00%	13.405%
15	9.619	656	659	662	rBV2	169590	273073	3.38%	0.454%
16	9.905	682	684	687	rVB	2809916	2497097	30.95%	4.148%
17	10.294	708	718	719	rBV3	121679	494470	6.13%	0.821%
18	10.339	720	722	724	rVB2	83945	116429	1.44%	0.193%
19	10.556	738	741	743	rBV4	47853	92514	1.15%	0.154%
20	10.694	750	753	756	rBV2	4041142	5313134	65.84%	8.827%
21	10.808	761	763	768	rVB2	192798	357042	4.42%	0.593%
22	11.265	800	803	804	rBV2	96054	162504	2.01%	0.270%
23	11.391	811	814	816	rBV	2966888	2468883	30.60%	4.101%
24	11.608	831	833	835	rBV	67692	110006	1.36%	0.183%
25	12.111	874	877	879	rBV2	136665	228539	2.83%	0.380%
26	12.979	950	953	956	rVB	5895557	6808806	84.38%	11.311%
27	13.882	1029	1032	1035	rVB	157825	251077	3.11%	0.417%
28	14.020	1042	1044	1047	rVB	1517078	2043780	25.33%	3.395%
29	14.534	1088	1089	1094	rVB3	88061	87248	1.08%	0.145%
30	14.660	1098	1100	1107	rVB2	55642	96763	1.20%	0.161%
31	15.460	1167	1170	1172	rBV	1083827	1548019	19.18%	2.572%
32	16.397	1249	1252	1258	rVB2	56008	131817	1.63%	0.219%

LSC Area Percent Report

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Data File : BF084300.D
Acq On : 6 Jan 2016 20:10
Operator : SJ/UM
Sample : H1017-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

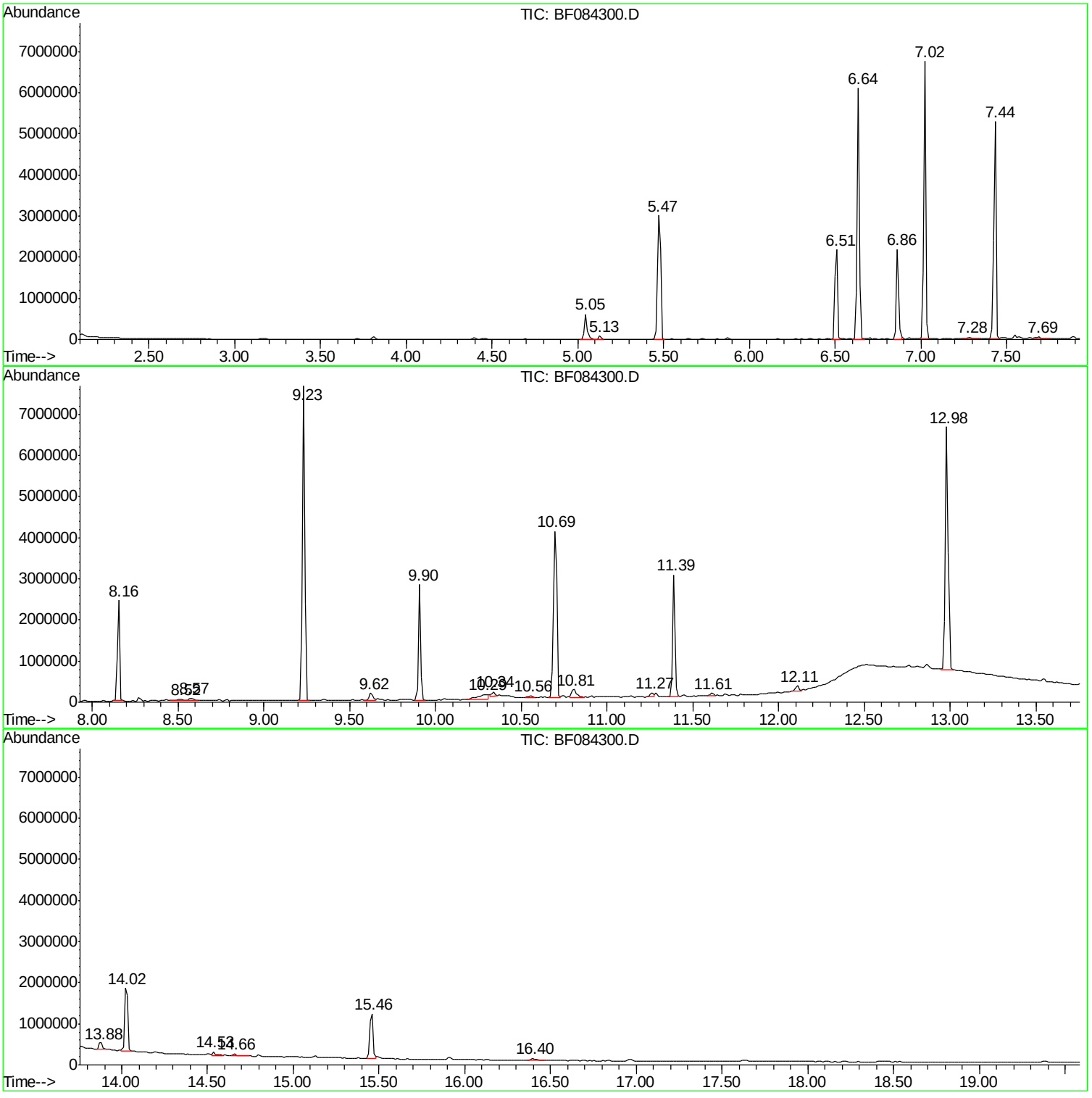
Sum of corrected areas: 60195243

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
Data File : BF084300.D
Acq On : 6 Jan 2016 20:10
Operator : SJ/UM
Sample : H1017-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
Data File : BF084300.D
Acq On : 6 Jan 2016 20:10
Operator : SJ/UM
Sample : H1017-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

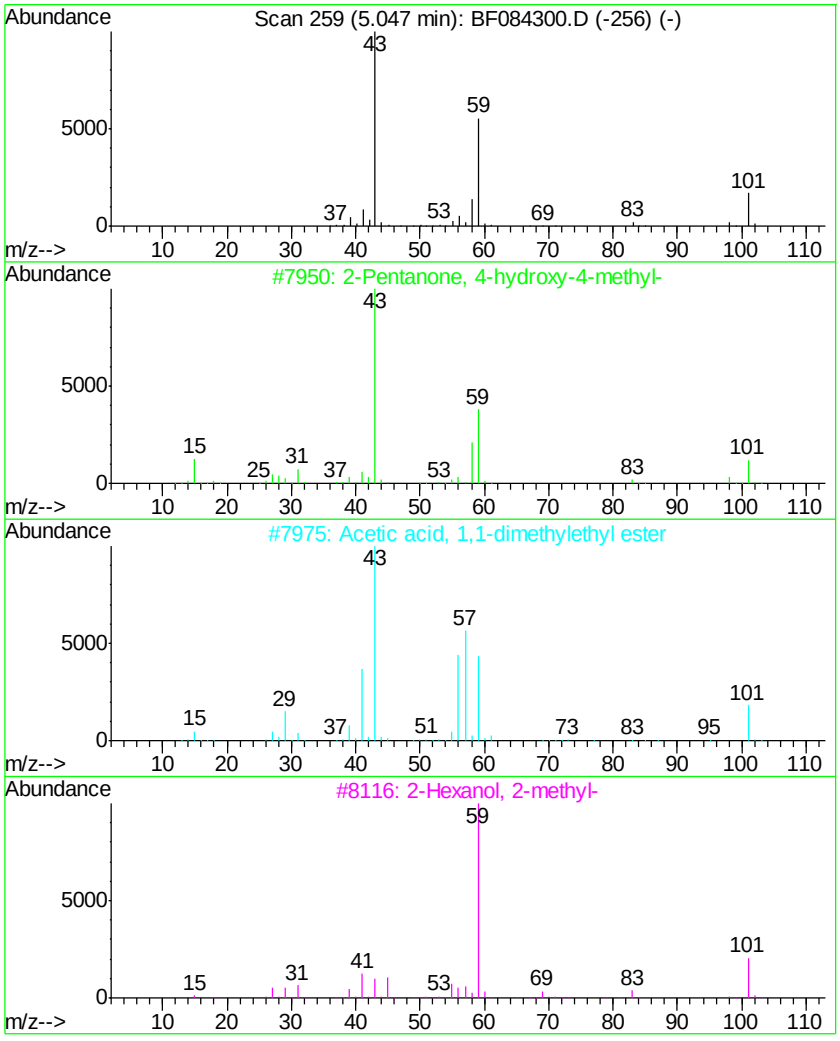
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

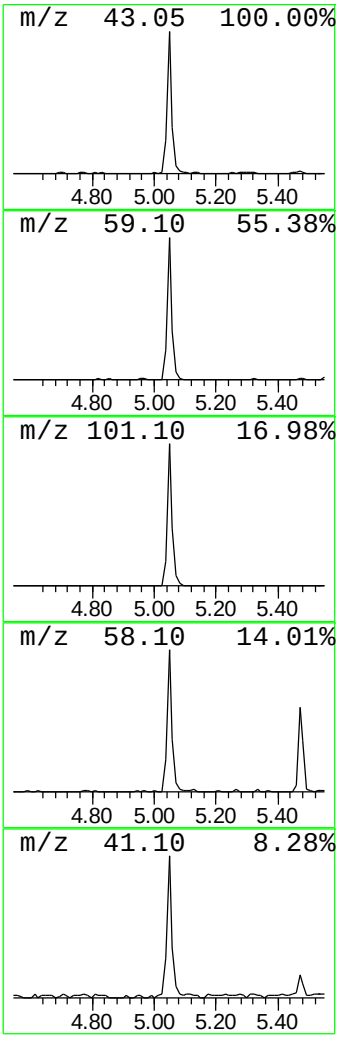
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	7.69 ng	694607	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
Data File : BF084300.D
Acq On : 6 Jan 2016 20:10
Operator : SJ/UM
Sample : H1017-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

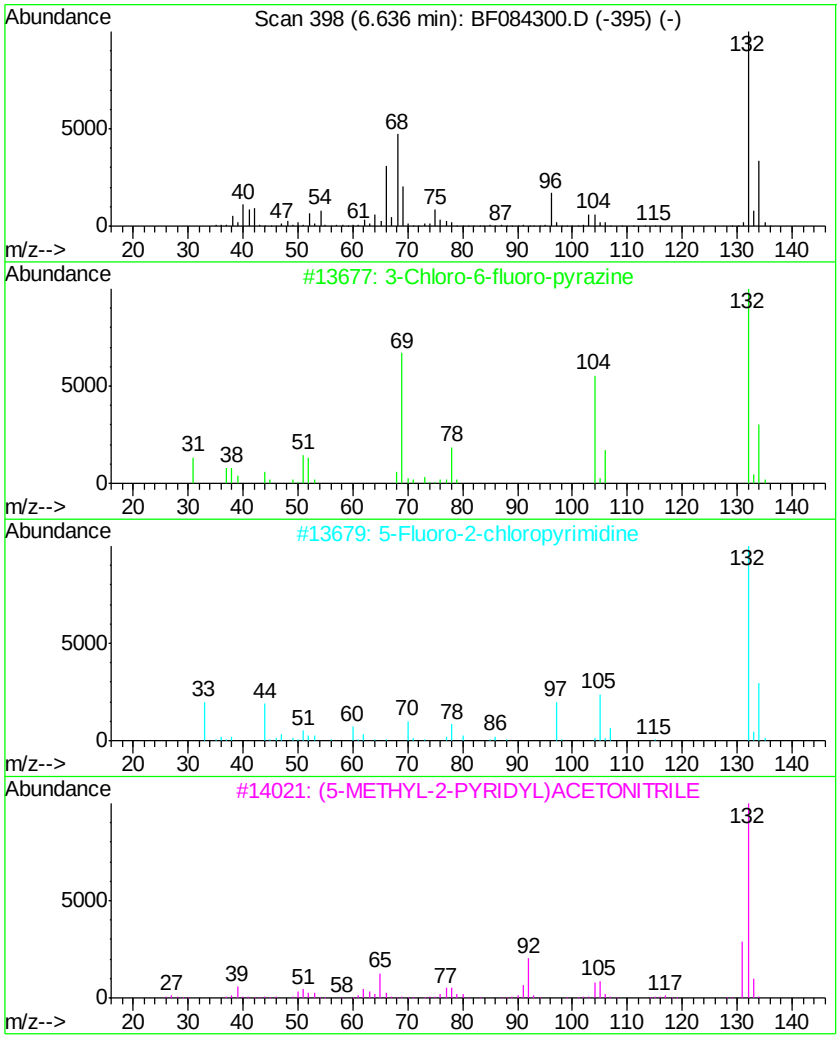
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

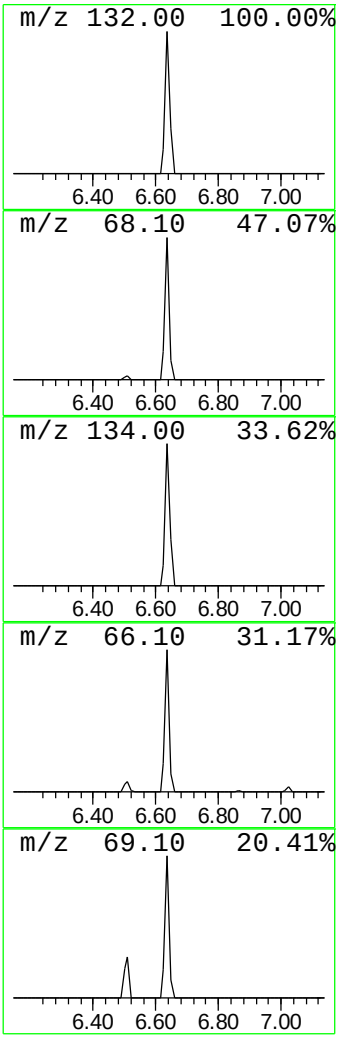
****

Peak Number 2 unknown6.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	65.02 ng	5875930	1,4-Dichlorobenzene-d4	6.86

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-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
Data File : BF084300.D
Acq On : 6 Jan 2016 20:10
Operator : SJ/UM
Sample : H1017-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

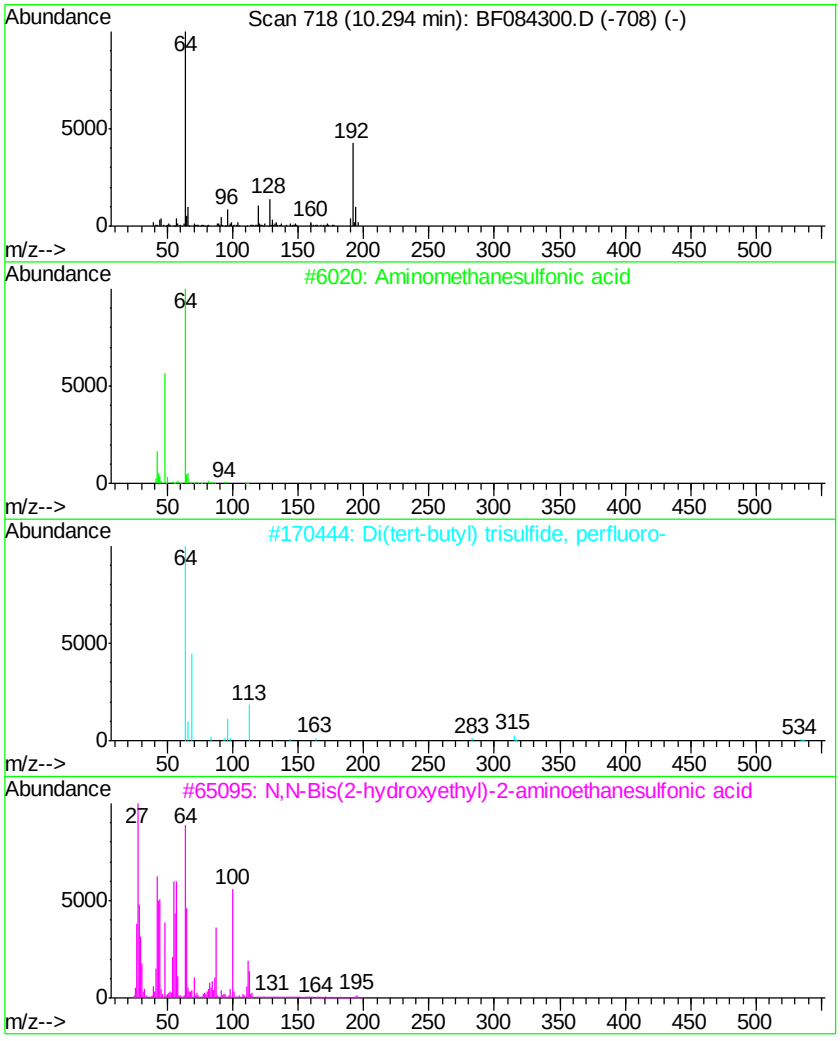
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

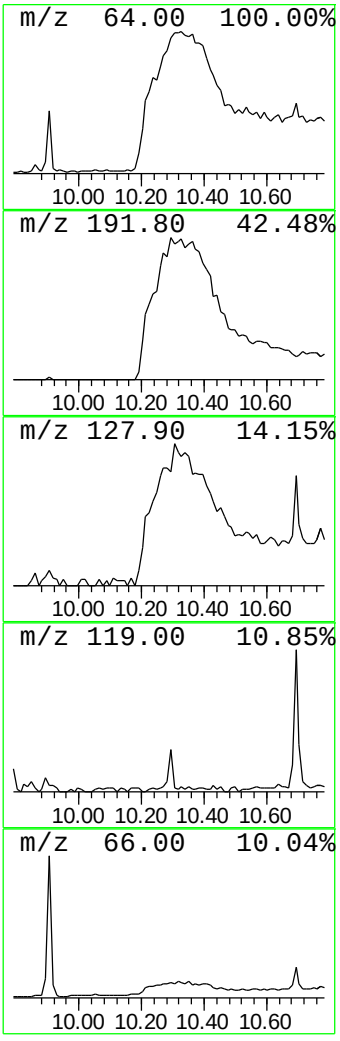
****

Peak Number 4 unknown10.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.29	3.96 ng	494470	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	39
2	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	39
3	N,N-Bis(2-hydroxyethyl)-2-aminoe...	213	C6H15NO5S	010191-18-1	38
4	Sulfur dioxide	64	O2S	007446-09-5	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
Data File : BF084300.D
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Sample : H1017-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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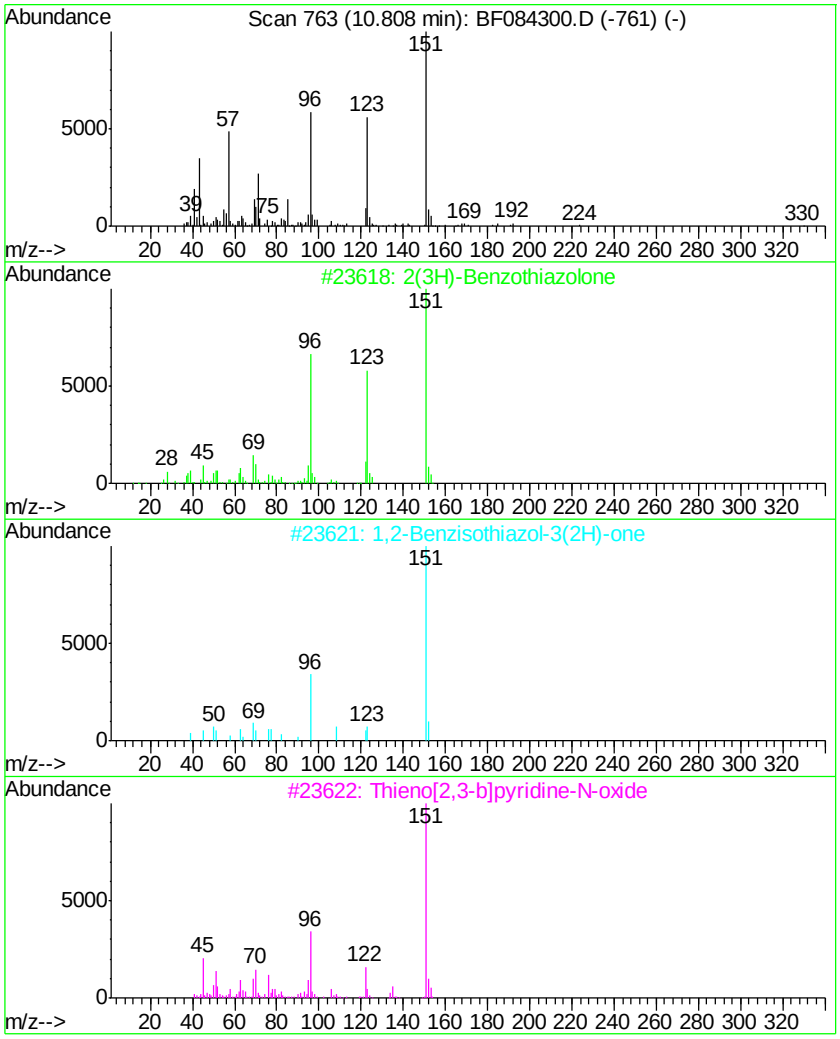
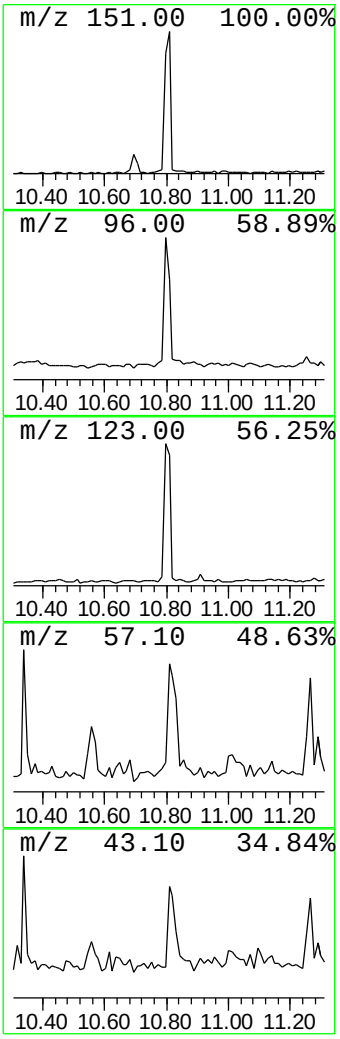
Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.89 ng	357042	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	91
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	50
3	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	38
4	2-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057351-75-4	35
5	2-Aminothiazolo(5,4-b)pyridine	151	C6H5N3S	031784-70-0	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010616\
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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-27

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

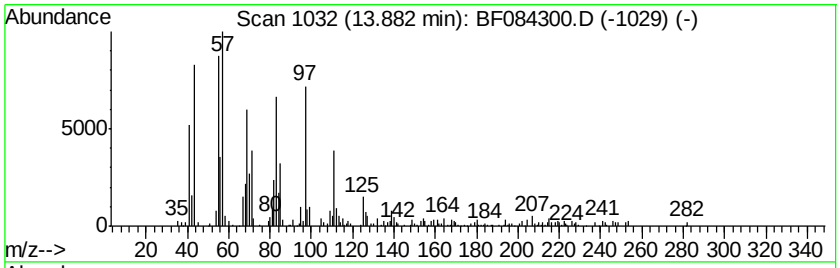
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

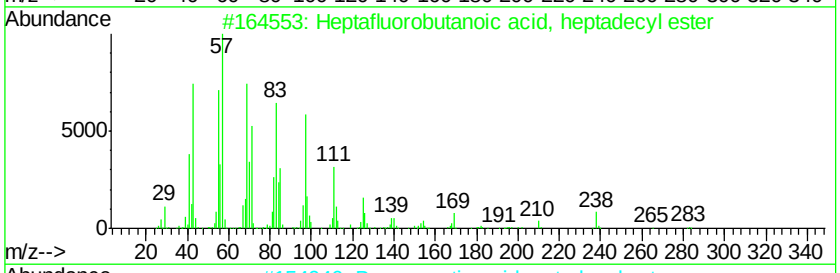
****

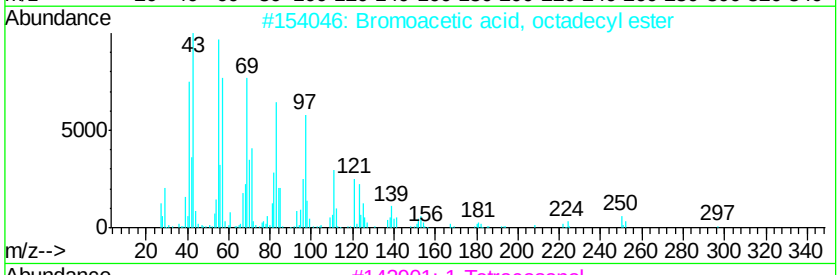
Peak Number 6 Heptafluorobutanoic acid, h... Concentration Rank 6

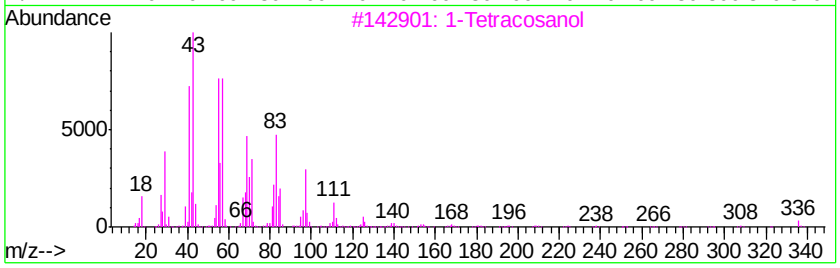
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	2.46 ng	251077	Chrysene-d12	14.03

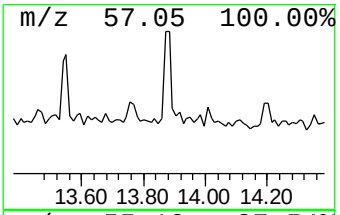
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	74
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	72
3	1-Tetracosanol	354	C24H50O	000506-51-4	58
4	1-Hexacosanol	382	C26H54O	000506-52-5	58
5	17-Pentatriacontene	491	C35H70	006971-40-0	52

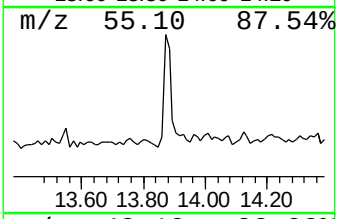


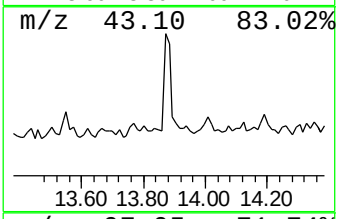


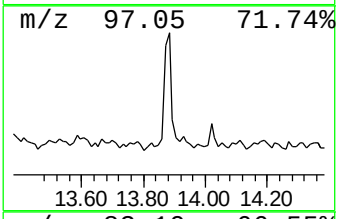


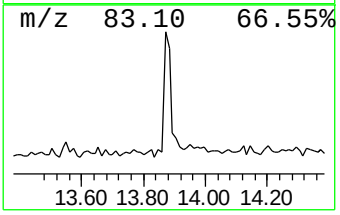












Tentatively Identified Compound (LSC) summary

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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...	5.05	7.7	ng	694607	1	6.86	1807390	20.0
unknown6.64	6.64	65.0	ng	5875930	1	6.86	1807390	20.0
unknown10.29	10.29	4.0	ng	494470	3	9.90	2497100	20.0
2(3H)-Benzothiazo...	10.81	2.9	ng	357042	4	11.39	2468880	20.0
Heptafluorobutano...	13.88	2.5	ng	251077	5	14.03	2043780	20.0