LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
Data File : BF091581.D
Acq On : 14 Dec 2016 13:01
Operator : UM/SJ
Sample : H5886-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VW-01

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-BF120916.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	4.956	249	251	254	rBV	662346	831006	11.23%	1.612%
2	5.401	287	290	292	rBV	2683499	3574144	48.30%	6.932%
3	6.430	378	380	383	rBV	2096588	2232482	30.17%	4.330%
4	6.567	389	392	394	rBV	6134846	5566010	75.22%	10.795%
5	6.796	410	412	415	rBV	1777448	1607431	21.72%	3.118%
6	6.956	423	426	428	rVB	6043822	5383054	72.75%	10.440%
7	7.367	459	462	464	rBV	4581130	4943613	66.81%	9.588%
8	8.087	522	525	527	rBV	2393827	2161159	29.21%	4.191%
9	9.059	605	610	612	rBV4	47641	75813	1.02%	0.147%
10	9.162	616	619	622	rBV	5605854	7399371	100.00%	14.351%
11	9.276	627	629	632	rVB4	38476	79878	1.08%	0.155%
12	9.345	634	635	639	rVV4	38088	79491	1.07%	0.154%
13	9.493	644	648	649	rBV3	61687	133964	1.81%	0.260%
14	9.562	652	654	655	rVB	164615	144567	1.95%	0.280%
15	9.699	663	666	667	rBV2	74689	123742	1.67%	0.240%
16	9.756	668	671	676	rVB	279153	569196	7.69%	1.104%
17	9.836	676	678	681	rBV	2039414	1982658	26.79%	3.845%
18	10.133	702	704	706	rVV2	61955	108262	1.46%	0.210%
19	10.453	730	732	735	rBV3	67735	157652	2.13%	0.306%
20	10.625	744	747	750	rBV	3434732	3611867	48.81%	7.005%
21	11.322	806	808	810	rBV	1951101	1692646	22.88%	3.283%
22	11.871	854	856	860	rBV2	560588	690621	9.33%	1.339%
23	12.659	923	925	929	rVB	729599	704599	9.52%	1.367%
24	12.911	944	947	950	rVB	4783235	4601853	62.19%	8.925%
25	13.814	1025	1026	1031	rVB2	125512	189915	2.57%	0.368%
26	13.962	1036	1039	1041	rBV	1118880	1385324	18.72%	2.687%
27	15.368	1160	1162	1165	rBV	931046	1440586	19.47%	2.794%
28	15.414	1165	1166	1173	rVB6	40684	89959	1.22%	0.174%

Sum of corrected areas: 51560863

LSC Report - Integrated Chromatogram

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Misc :
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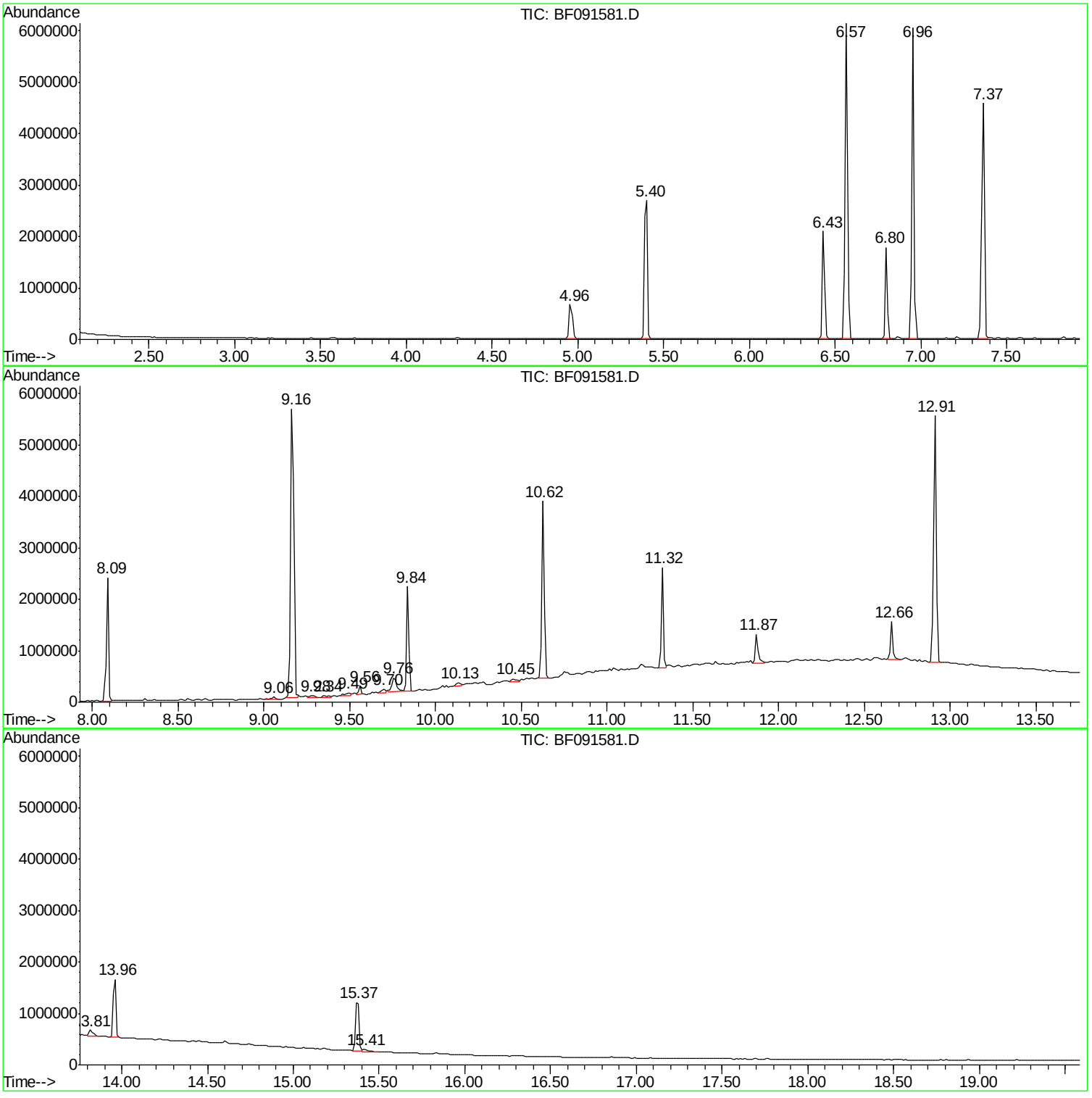
Instrument : BNA_F
ClientSampleId : VW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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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Misc :
ALS Vial : 34 Sample Multiplier: 1

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ClientSampleId : VW-01

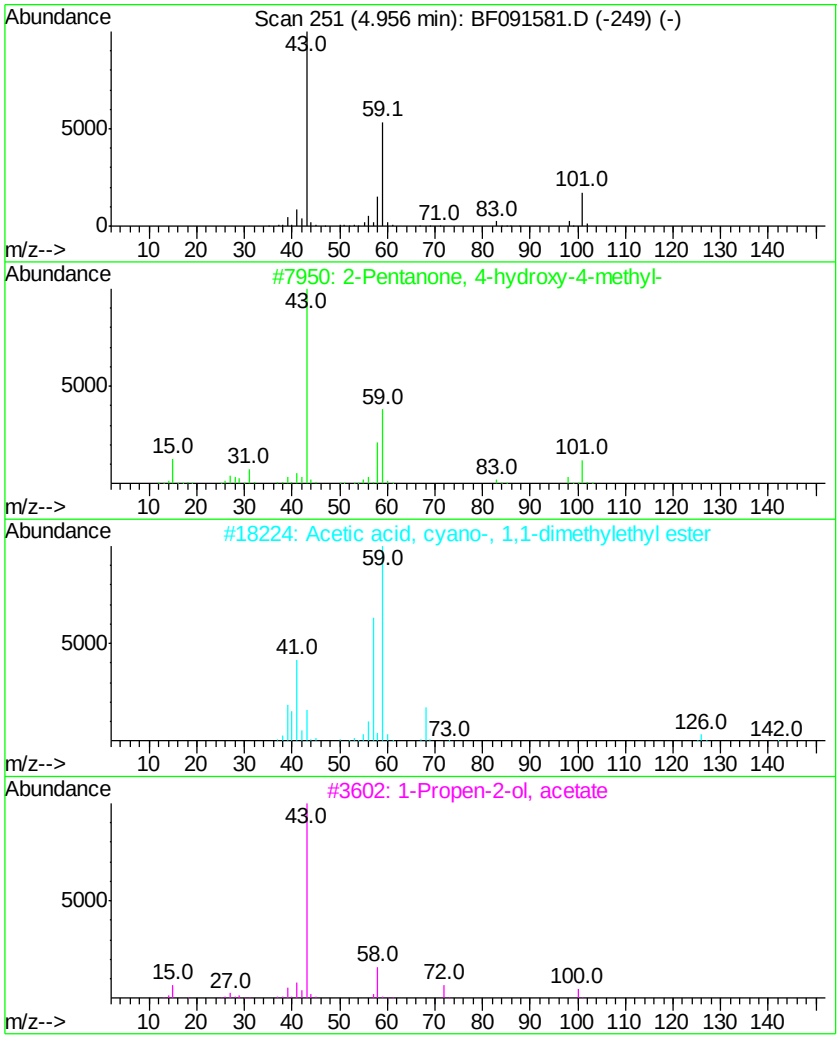
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

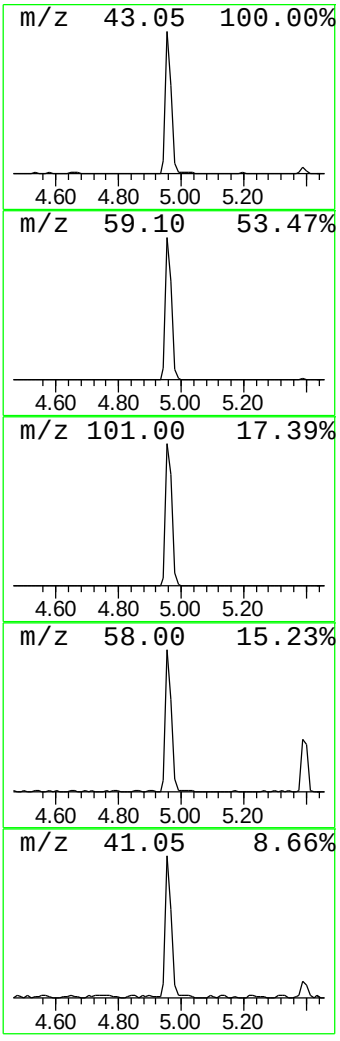
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	10.34 ng	831006	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_F
ClientSampleId : VW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

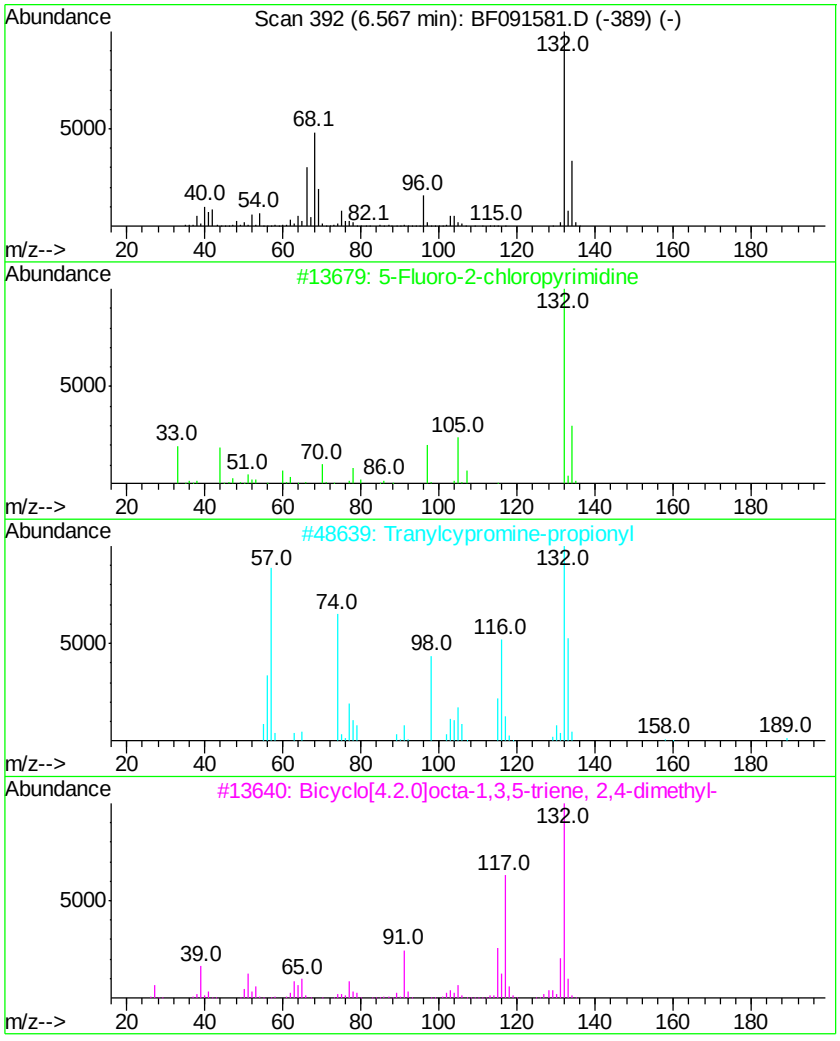
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

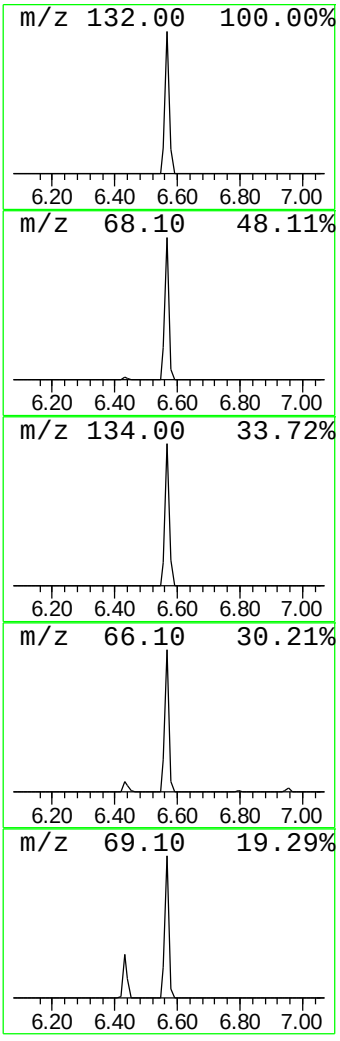
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	69.25 ng	5566010	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Data File : BF091581.D
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Operator : UM/SJ
Sample : H5886-02
Misc :
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Instrument : BNA_F
ClientSampleId : VW-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
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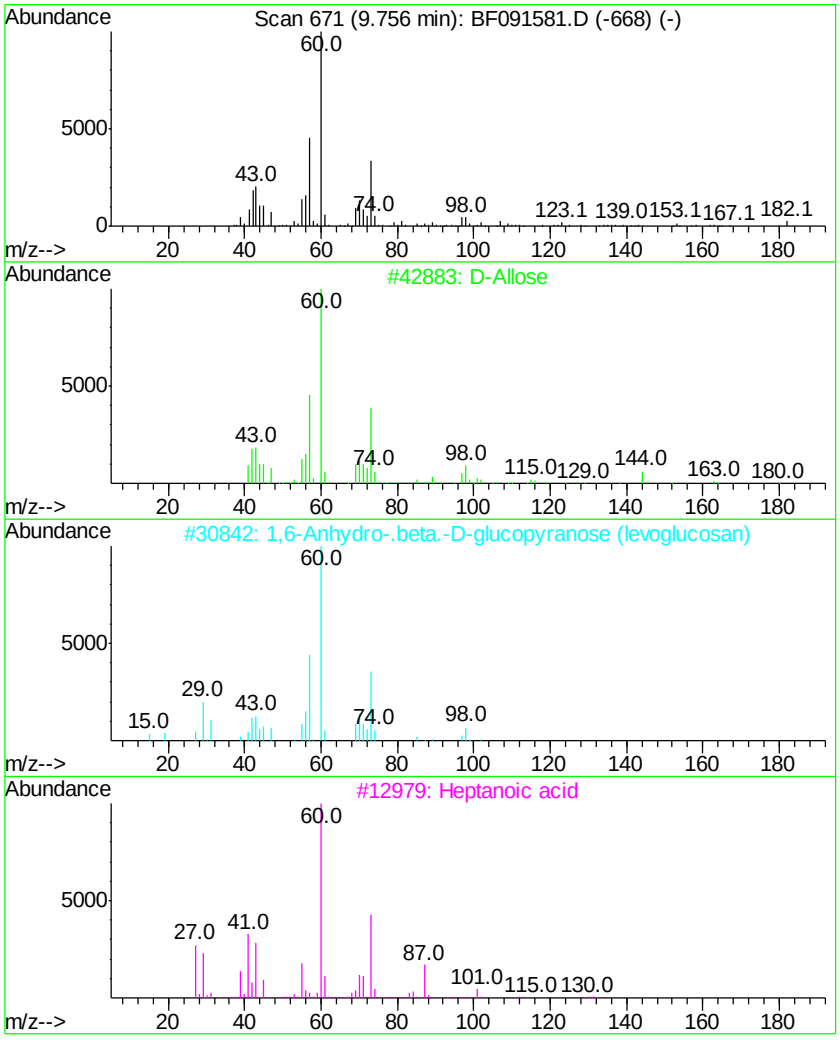
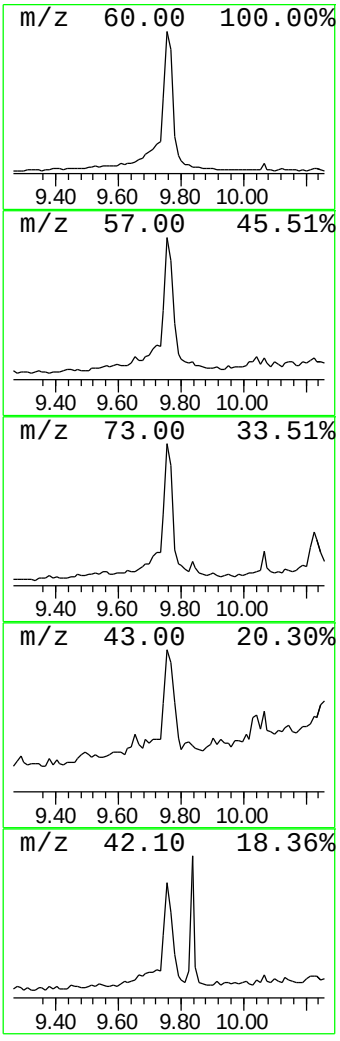
Peak Number 4 D-Allose Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	5.74 ng	569196	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	90
2	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	86
3	Heptanoic acid	130	C7H14O2	000111-14-8	59
4	Pentanoic acid	102	C5H10O2	000109-52-4	53
5	Butanoic acid	88	C4H8O2	000107-92-6	50





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Sample : H5886-02
Misc :
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Instrument : BNA_F
ClientSampleId : VW-01

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TIC Library : C:\DATABASE\NIST02.L
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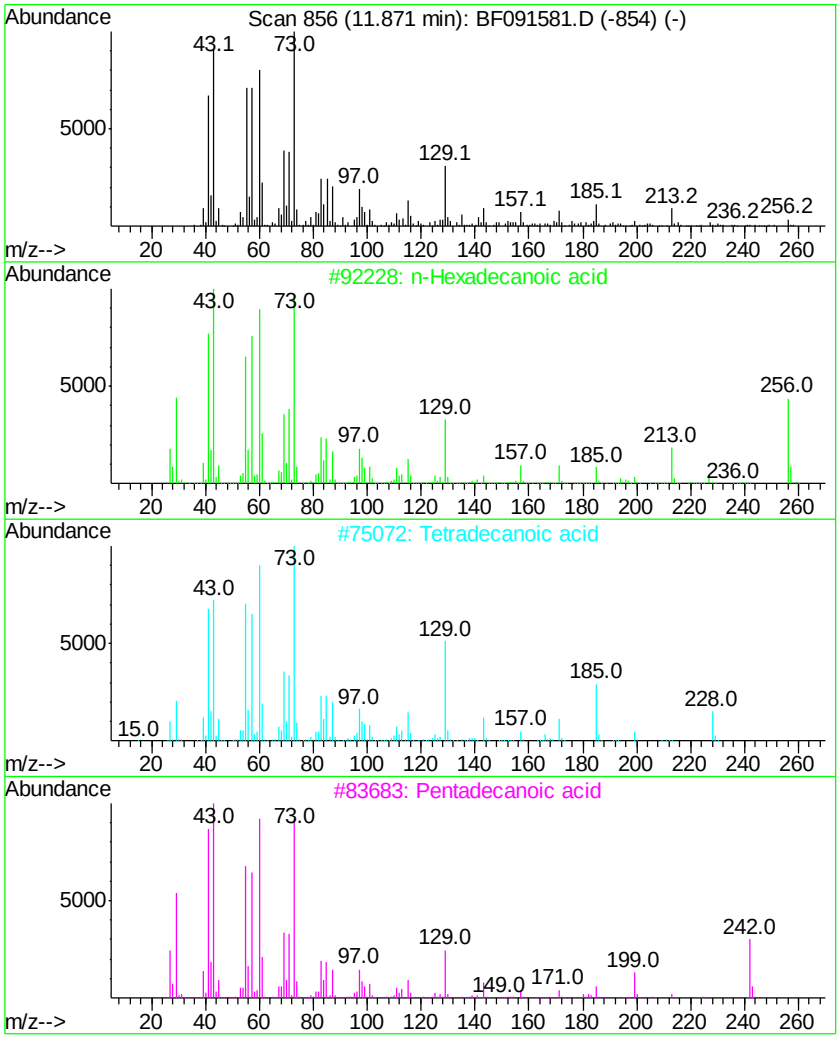
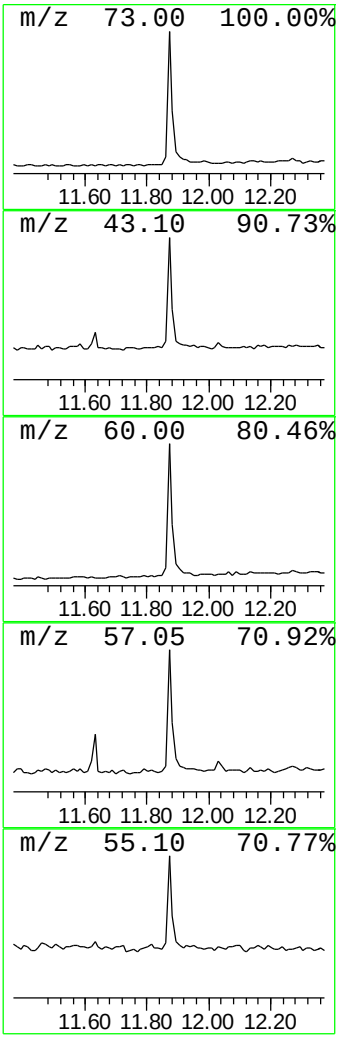
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	8.16 ng	690621	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tridecane	184	C13H28	000629-50-5	25
5	Octacosane	394	C28H58	000630-02-4	11





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Sample : H5886-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VW-01

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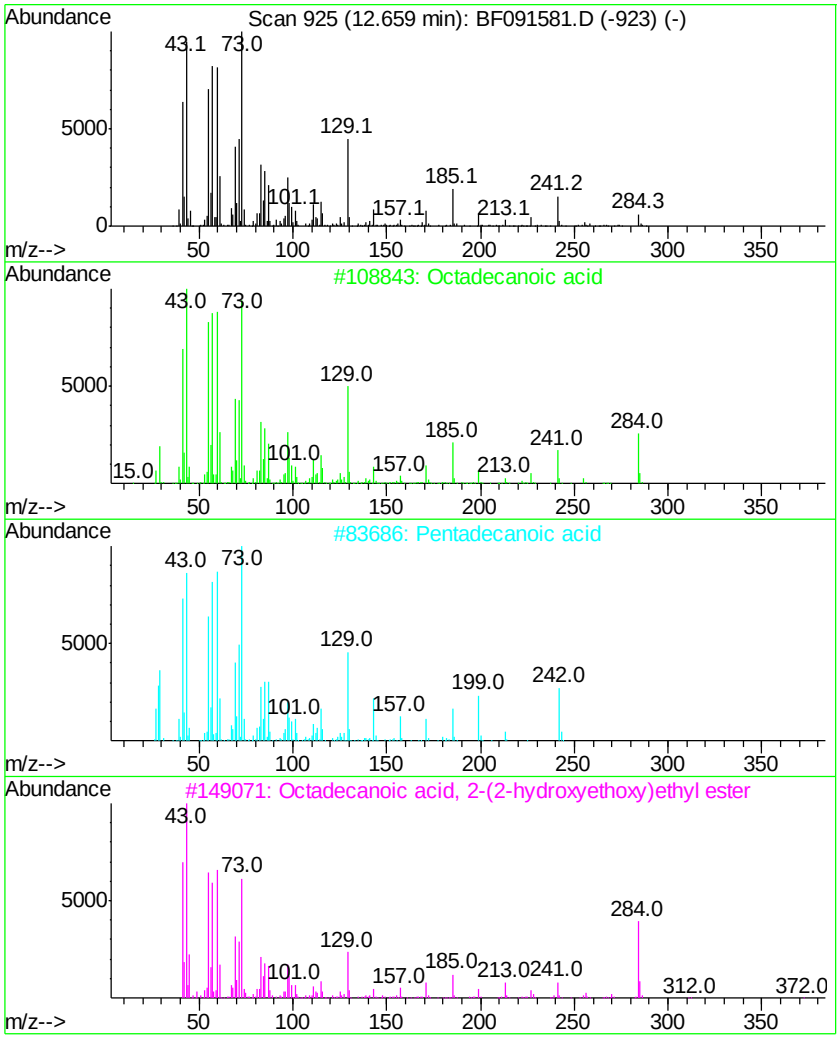
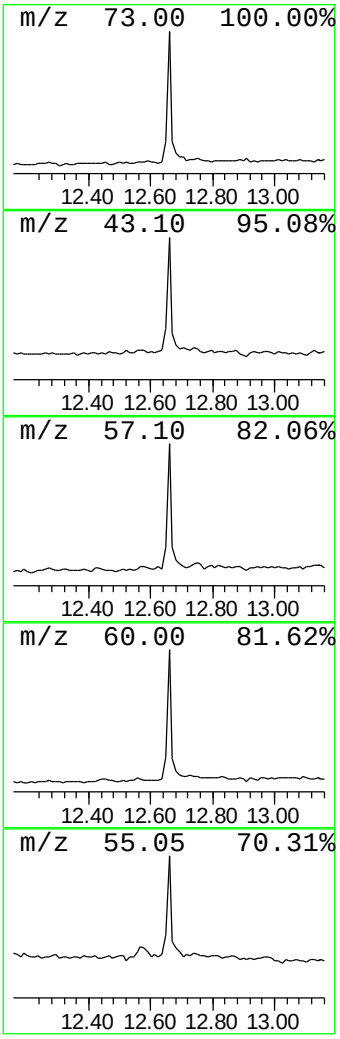
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	10.17 ng	704599	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : VW-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

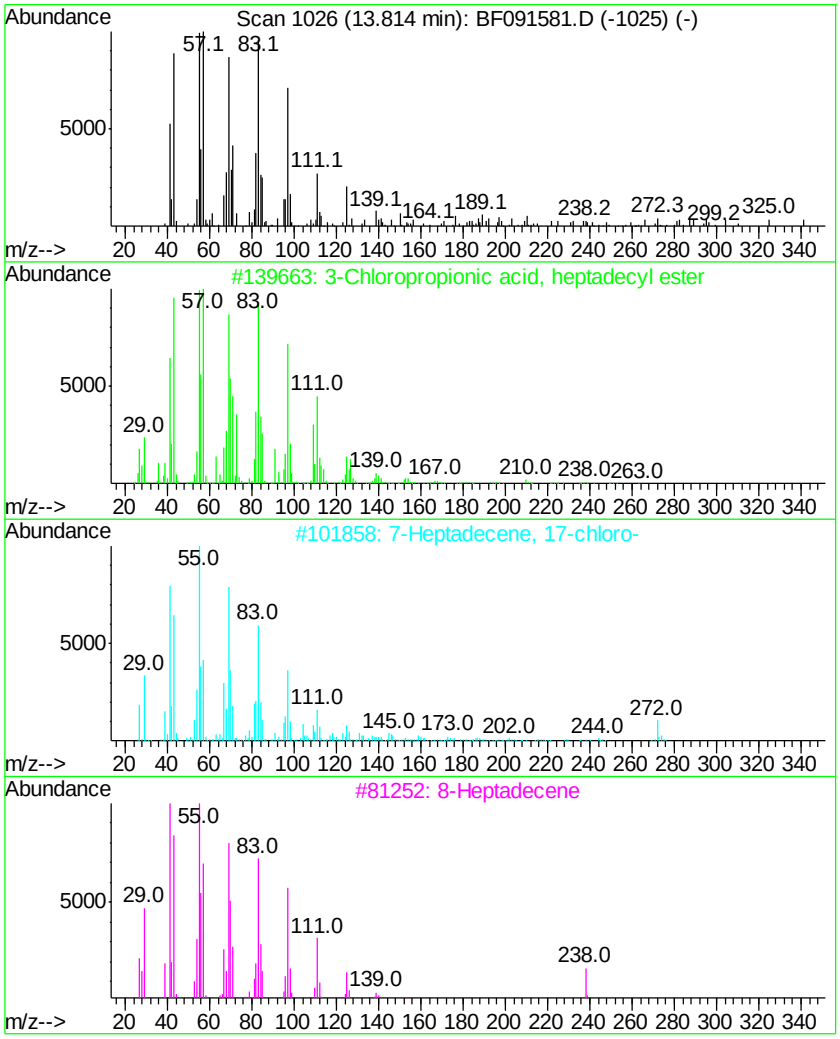
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

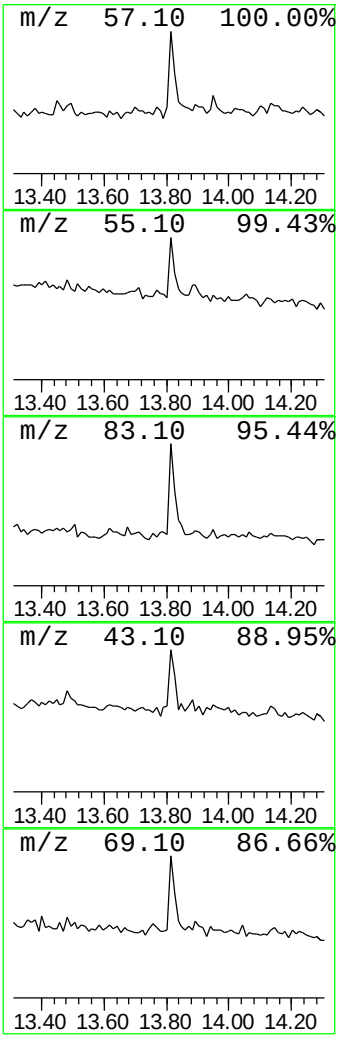
****

Peak Number 7 3-Chloropropionic acid, hep... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.74 ng	189915	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2	7-Heptadecene, 17-chloro-	272	C17H33Cl	056554-79-1	90
3	8-Heptadecene	238	C17H34	054290-12-9	83
4	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	78
5	1-Nonadecene	266	C19H38	018435-45-5	78





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...	4.96	10.3	ng	831006	1	6.80	1607430	20.0
unknown6.57	6.57	69.3	ng	5566010	1	6.80	1607430	20.0
D-Allose	9.76	5.7	ng	569196	3	9.84	1982660	20.0
n-Hexadecanoic acid	11.87	8.2	ng	690621	4	11.32	1692650	20.0
Octadecanoic acid	12.66	10.2	ng	704599	5	13.96	1385320	20.0
3-Chloropropionic...	13.81	2.7	ng	189915	5	13.96	1385320	20.0