LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109123.D
Acq On : 19 Sep 2018 4:15
Operator : JU/SJ
Sample : J4930-07
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-D-S

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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	4.901	432	436	450	rVB	142137	150296	4.70%	0.789%
2	5.325	504	508	519	rBV	1078321	985663	30.83%	5.177%
3	6.348	678	682	695	rBV	806657	683104	21.37%	3.588%
4	6.490	702	706	709	rBV	1966079	1647200	51.52%	8.651%
5	6.719	742	745	749	rBV	727136	604431	18.91%	3.174%
6	6.878	768	772	775	rBV	2654052	2265705	70.87%	11.899%
7	7.284	836	841	844	rBV	1876445	1760093	55.06%	9.244%
8	8.001	959	963	977	rBV	809126	646752	20.23%	3.397%
9	9.078	1142	1146	1149	rBV	3234869	2767019	86.55%	14.532%
10	9.472	1210	1213	1219	rBV	96673	83102	2.60%	0.436%
11	9.748	1257	1260	1272	rVB	674738	611916	19.14%	3.214%
12	10.536	1390	1394	1408	rBV	1234265	1181107	36.94%	6.203%
13	11.225	1508	1511	1515	rBV	656145	609223	19.06%	3.200%
14	12.813	1777	1781	1784	rBV	3429851	3196944	100.00%	16.790%
15	13.719	1930	1935	1948	rBV2	71545	122155	3.82%	0.642%
16	13.854	1954	1958	1965	rBV	979325	824581	25.79%	4.331%
17	14.636	2088	2091	2095	rBV	32590	35142	1.10%	0.185%
18	14.707	2099	2103	2107	rVB	79251	74198	2.32%	0.390%
19	14.954	2142	2145	2149	rBV	44364	45095	1.41%	0.237%
20	15.260	2192	2197	2202	rBV	544901	632511	19.78%	3.322%
21	15.313	2202	2206	2210	rVB	46915	57500	1.80%	0.302%
22	15.713	2270	2274	2279	rBV	38126	56788	1.78%	0.298%

Sum of corrected areas: 19040525

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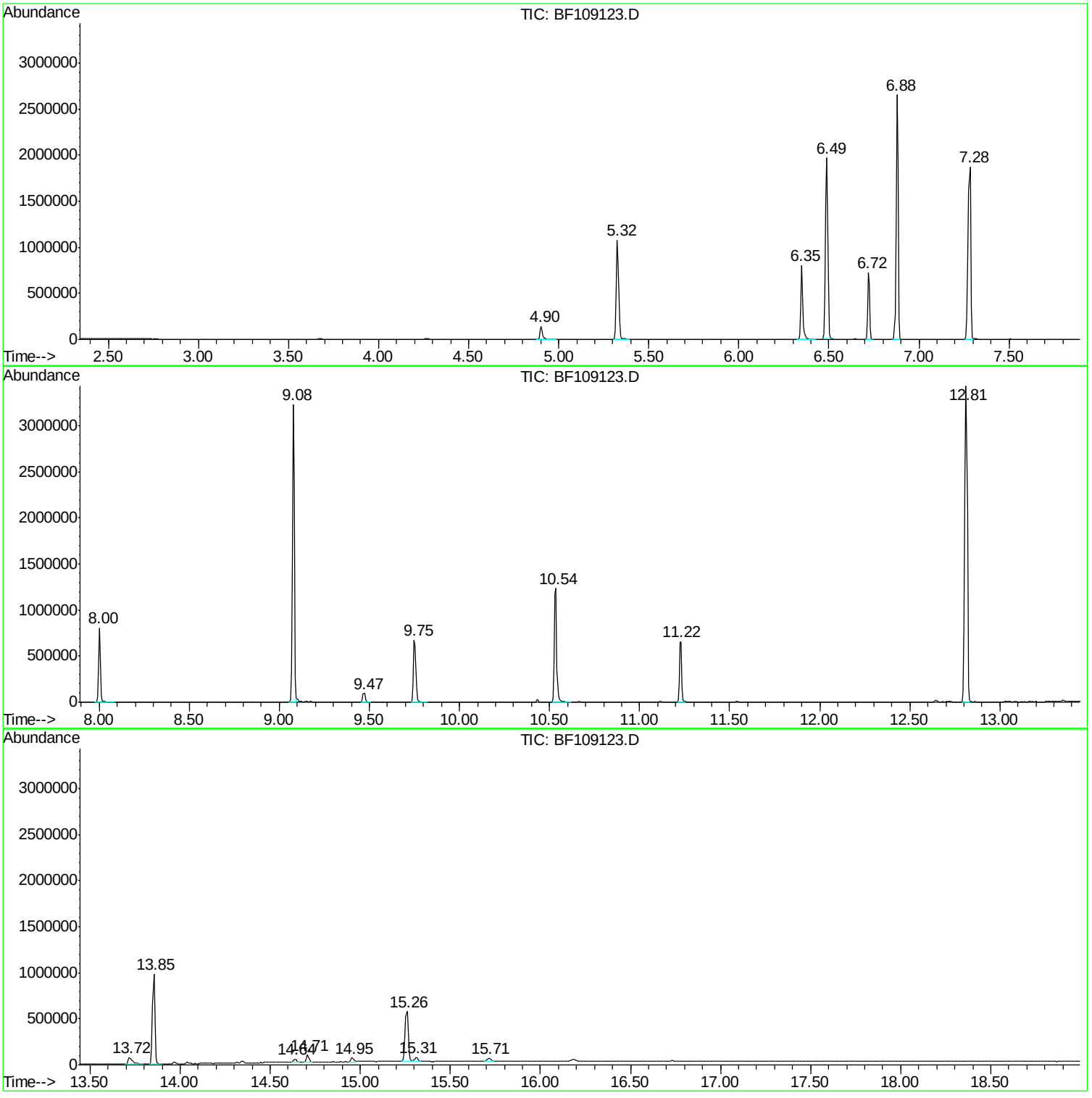
ClientSampleId :
091318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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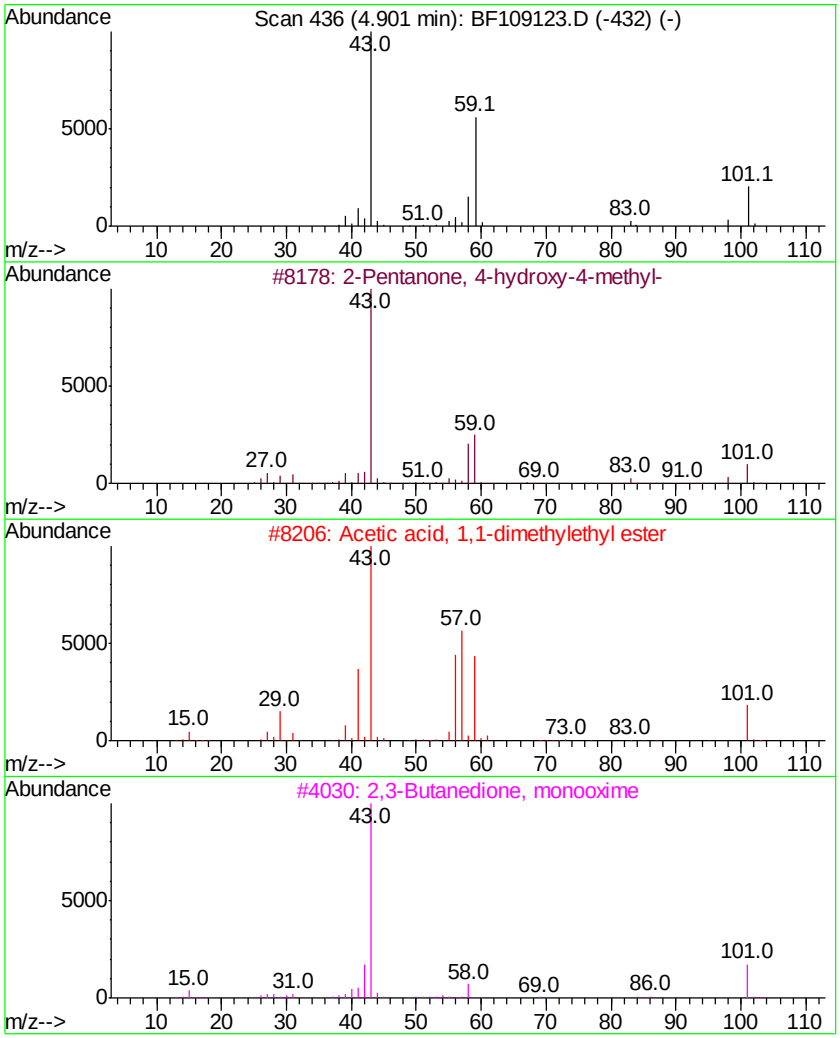
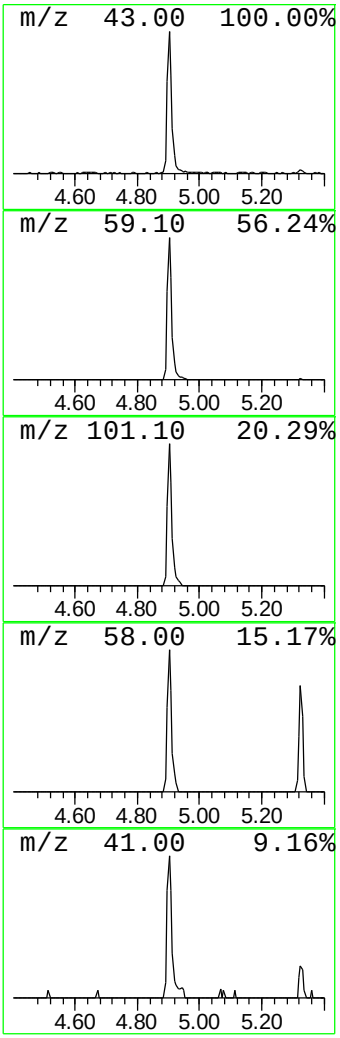
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	4.97 ng	150296	1,4-Dichlorobenzene-d4	6.72

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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
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Misc :
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Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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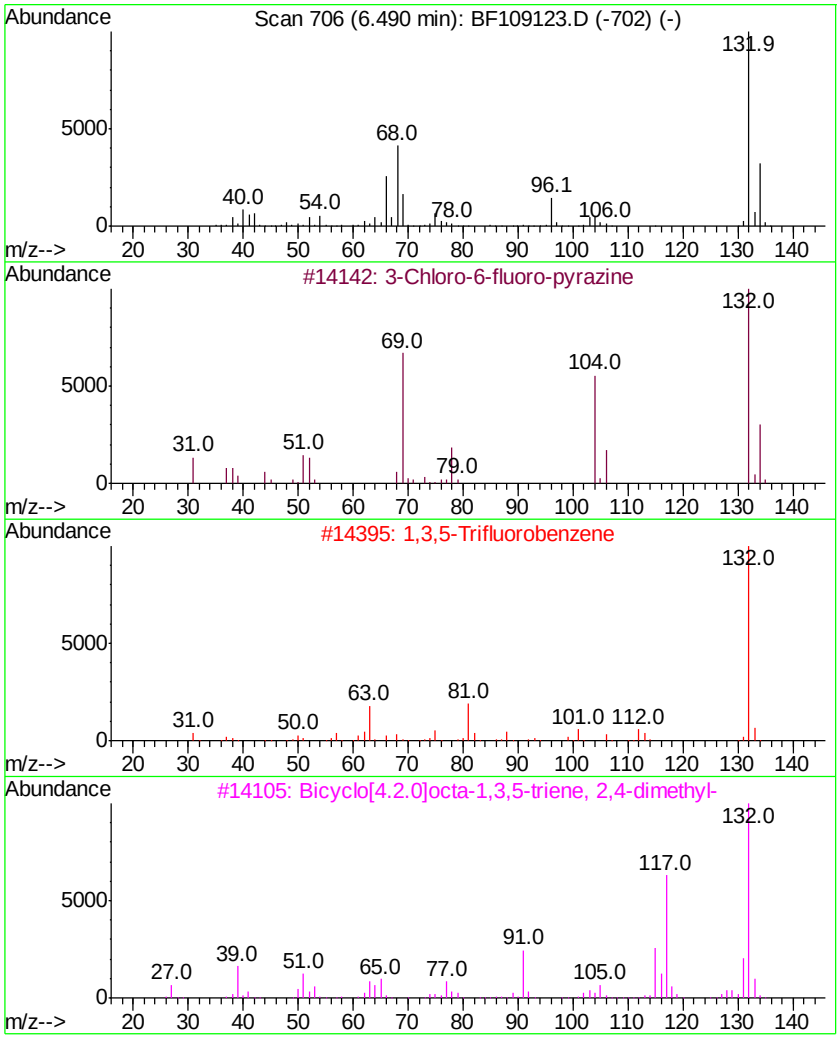
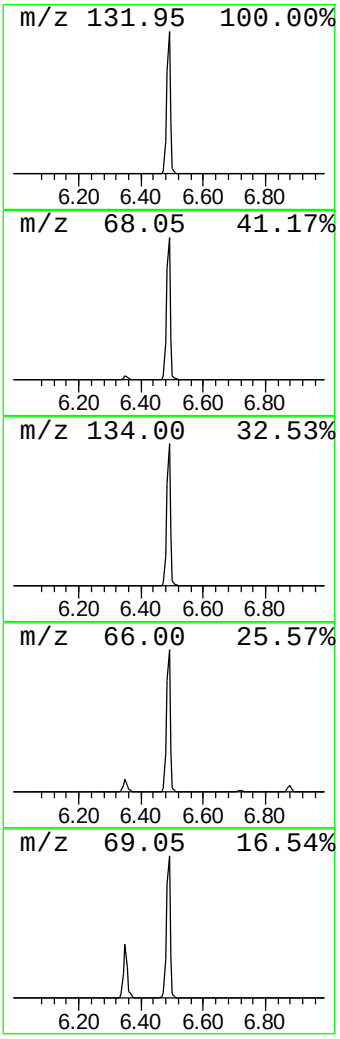
Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	54.50 ng	1647200	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





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Acq On : 19 Sep 2018 4:15
Operator : JU/SJ
Sample : J4930-07
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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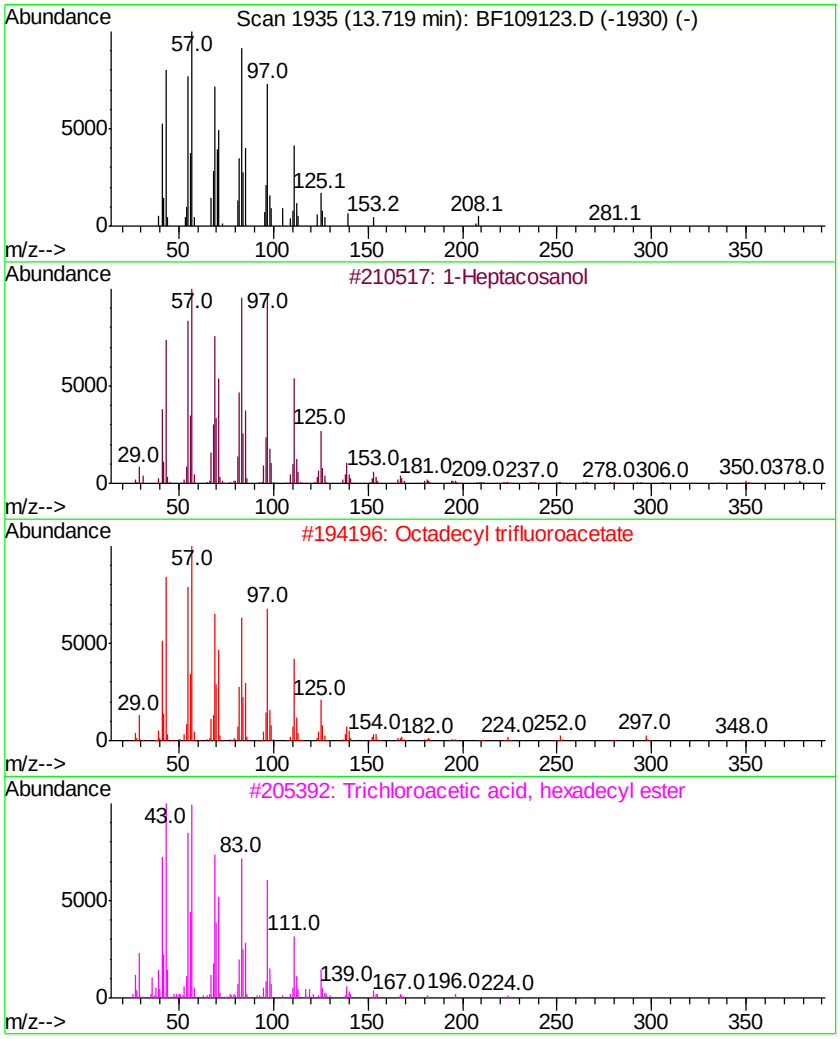
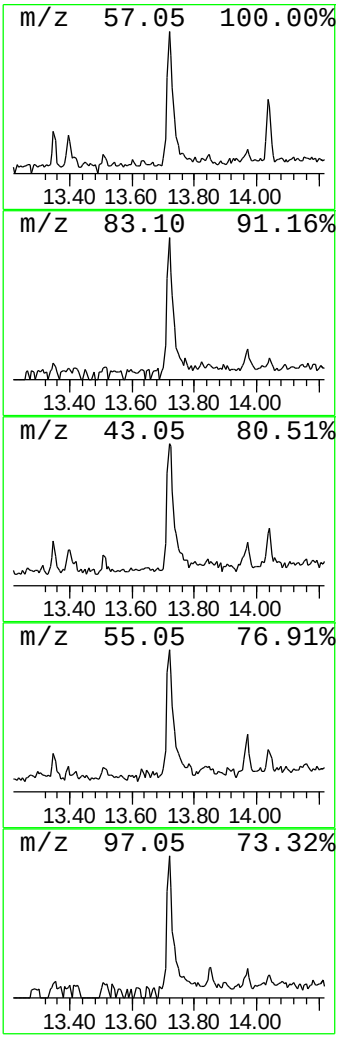
Peak Number 4 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.96 ng	122155	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4	1-Docosene	308	C22H44	001599-67-3	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





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Operator : JU/SJ
Sample : J4930-07
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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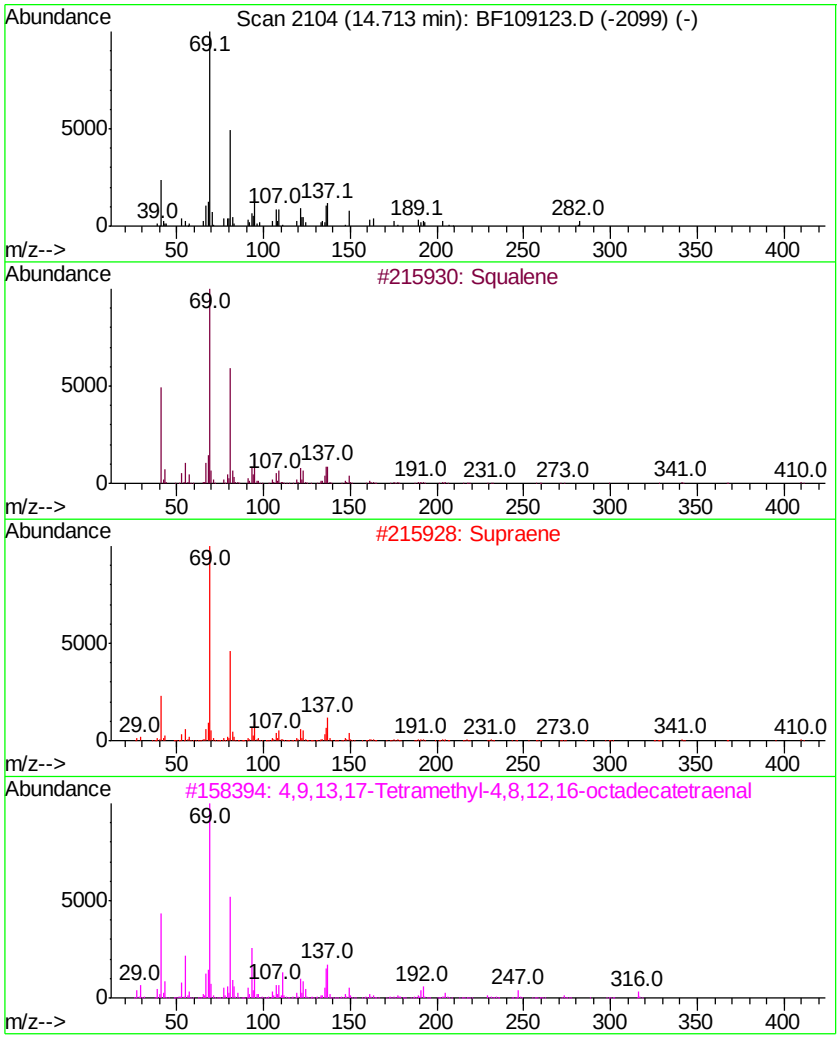
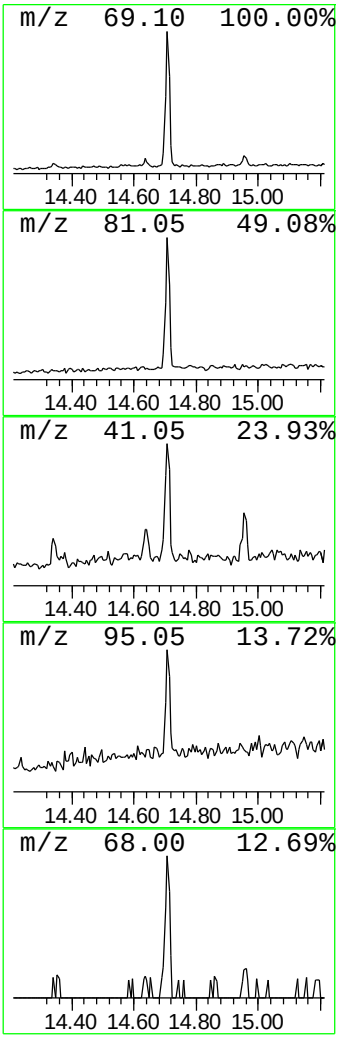
Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.35 ng	74198	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	87
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72





Tentatively Identified Compound (LSC) summary

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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	5.0	ng	150296	1	6.72	604431	20.0
unknown6.49	6.49	54.5	ng	1647200	1	6.72	604431	20.0
1-Heptacosanol	13.72	3.0	ng	122155	5	13.85	824581	20.0
Squalene	14.71	2.4	ng	74198	6	15.26	632511	20.0