LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108249.D
Acq On : 17 Aug 2018 17:59
Operator : JU/SJ
Sample : J4500-21
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROCK

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-BF080818.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	5.254	491	496	506	rBV	556583	648737	18.57%	2.200%
2	5.642	557	562	565	rBV	3026194	2776401	79.48%	9.416%
3	6.636	725	731	741	rBV	2849928	2984112	85.43%	10.121%
4	6.784	752	756	759	rBV	3335977	2909298	83.29%	9.867%
5	7.013	792	795	799	rBV	1042146	868764	24.87%	2.947%
6	7.172	818	822	825	rBV	2880995	2302429	65.91%	7.809%
7	7.578	886	891	894	rBV	1964586	1855543	53.12%	6.293%
8	8.295	1010	1013	1017	rBV	1164781	1047611	29.99%	3.553%
9	9.372	1192	1196	1199	rBV	3960527	3349509	95.89%	11.360%
10	9.760	1259	1262	1265	rBV	198256	150609	4.31%	0.511%
11	10.060	1309	1313	1325	rBV	1330595	1163082	33.30%	3.945%
12	10.854	1443	1448	1460	rBV	1848608	1880681	53.84%	6.379%
13	11.554	1563	1567	1571	rBV	1307780	1134280	32.47%	3.847%
14	13.142	1832	1837	1840	rBV	3941449	3493055	100.00%	11.847%
15	14.054	1988	1992	2006	rVB2	83751	180961	5.18%	0.614%
16	14.207	2014	2018	2022	rBV	1291382	1217983	34.87%	4.131%
17	14.336	2038	2040	2045	rBV	34825	37936	1.09%	0.129%
18	14.648	2090	2093	2099	rBV2	49518	60961	1.75%	0.207%
19	14.977	2145	2149	2152	rVB2	45100	47954	1.37%	0.163%
20	15.059	2160	2163	2166	rVB	83457	82337	2.36%	0.279%
21	15.342	2207	2211	2215	rVB	53748	67065	1.92%	0.227%
22	15.771	2277	2284	2292	rBV	755804	1113620	31.88%	3.777%
23	16.236	2359	2363	2368	rBV2	43070	63119	1.81%	0.214%
24	16.789	2454	2457	2463	rVB3	29814	48545	1.39%	0.165%

Sum of corrected areas: 29484592

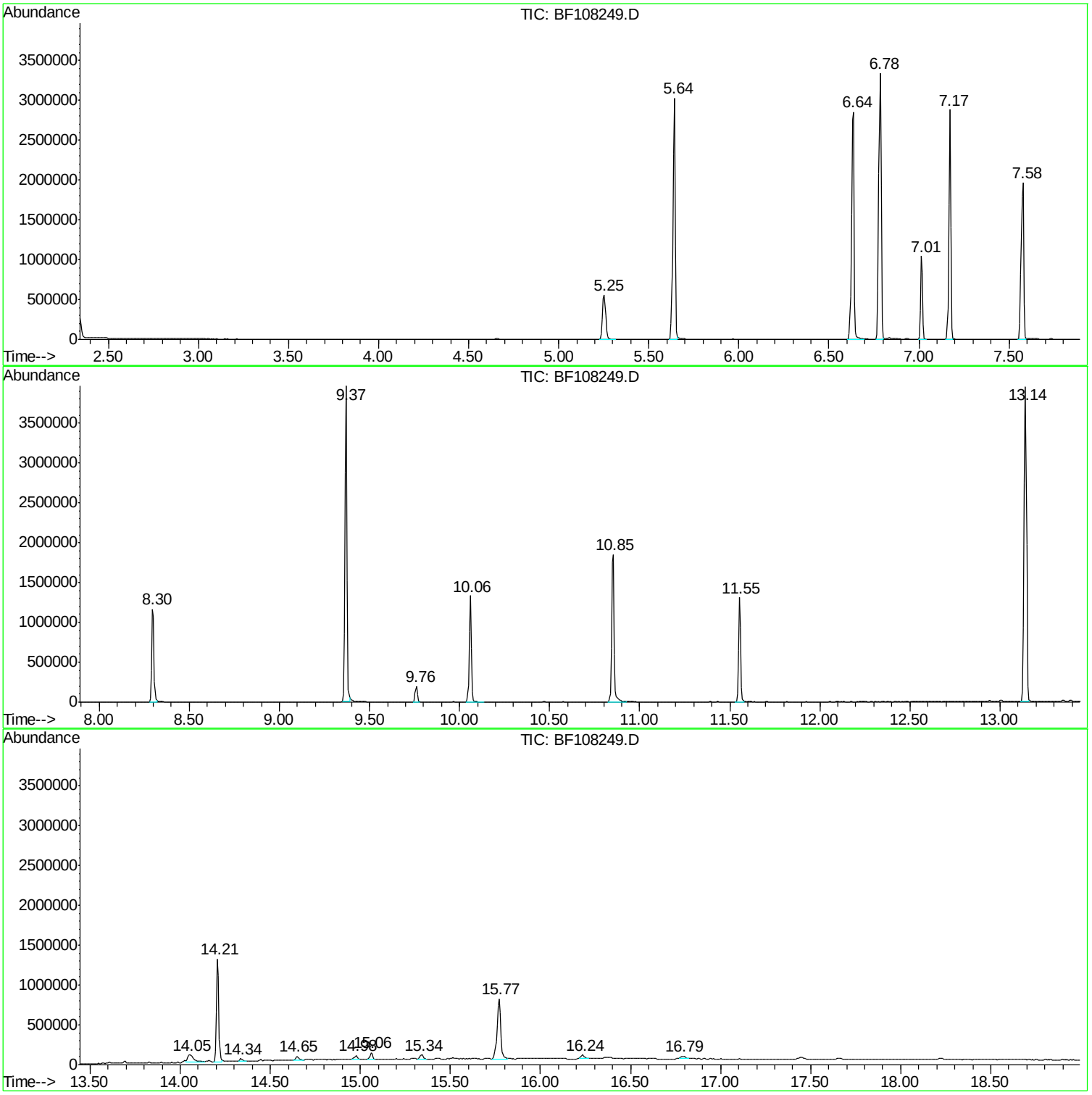
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108249.D
Acq On : 17 Aug 2018 17:59
Operator : JU/SJ
Sample : J4500-21
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROCK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108249.D
Acq On : 17 Aug 2018 17:59
Operator : JU/SJ
Sample : J4500-21
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROCK

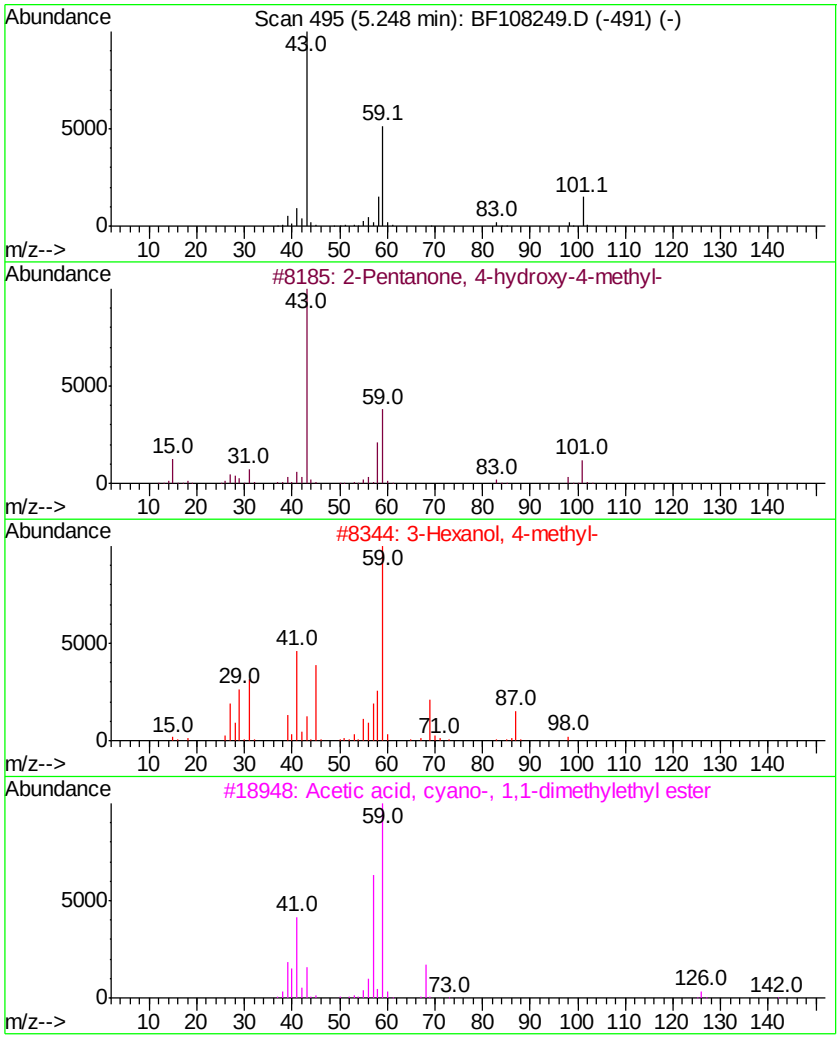
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

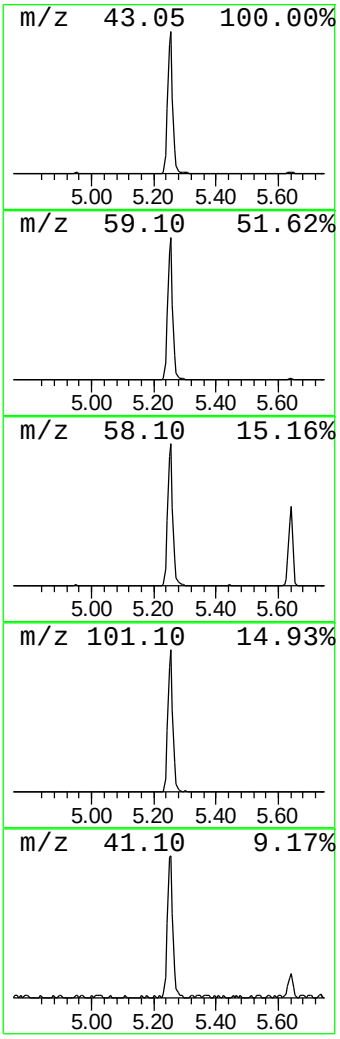
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	14.93 ng	648737	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108249.D
Acq On : 17 Aug 2018 17:59
Operator : JU/SJ
Sample : J4500-21
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROCK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

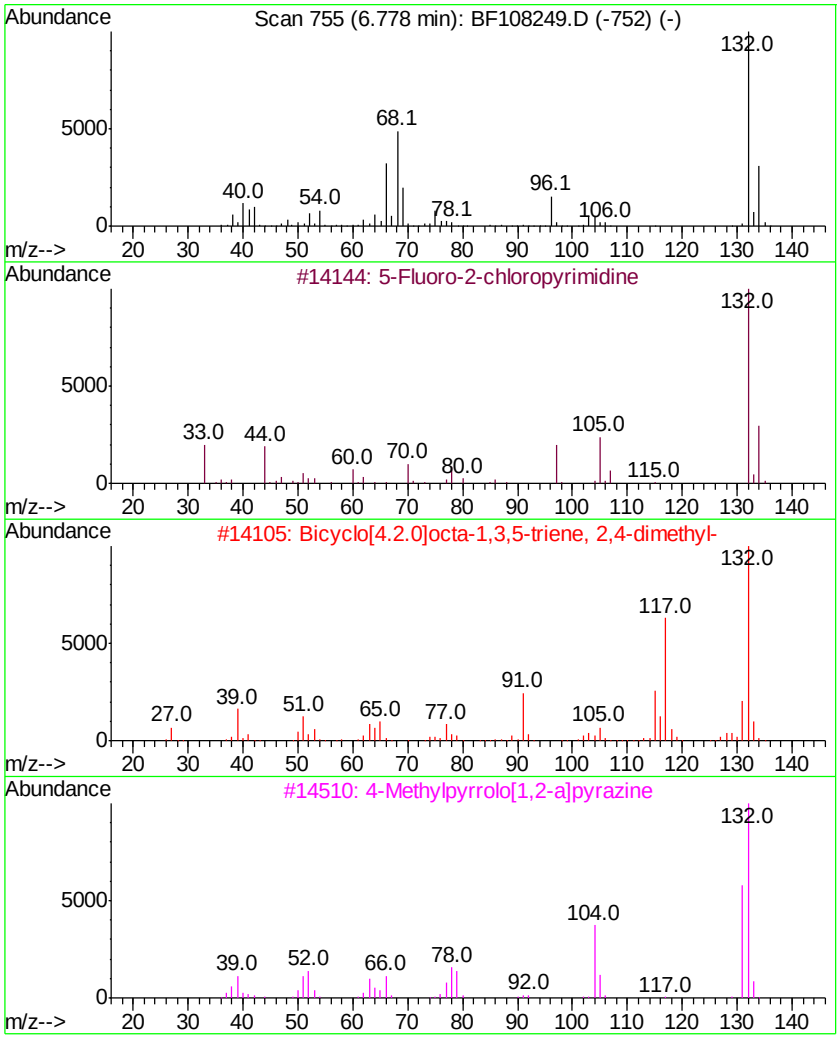
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

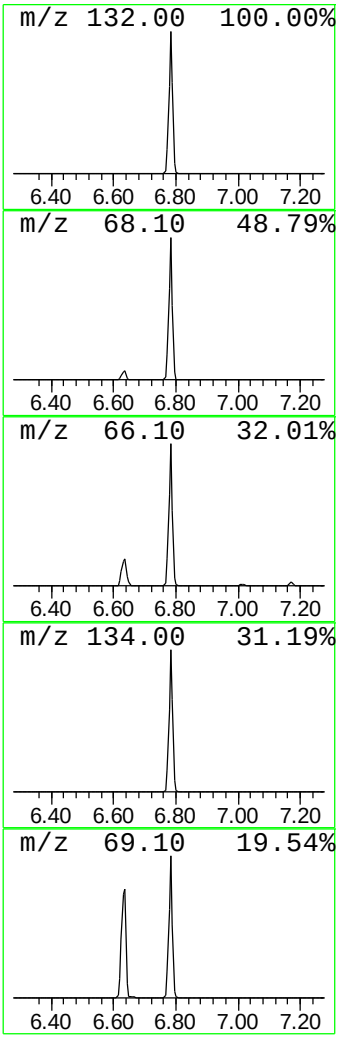
****

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	66.98 ng	2909300	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108249.D
Acq On : 17 Aug 2018 17:59
Operator : JU/SJ
Sample : J4500-21
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROCK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

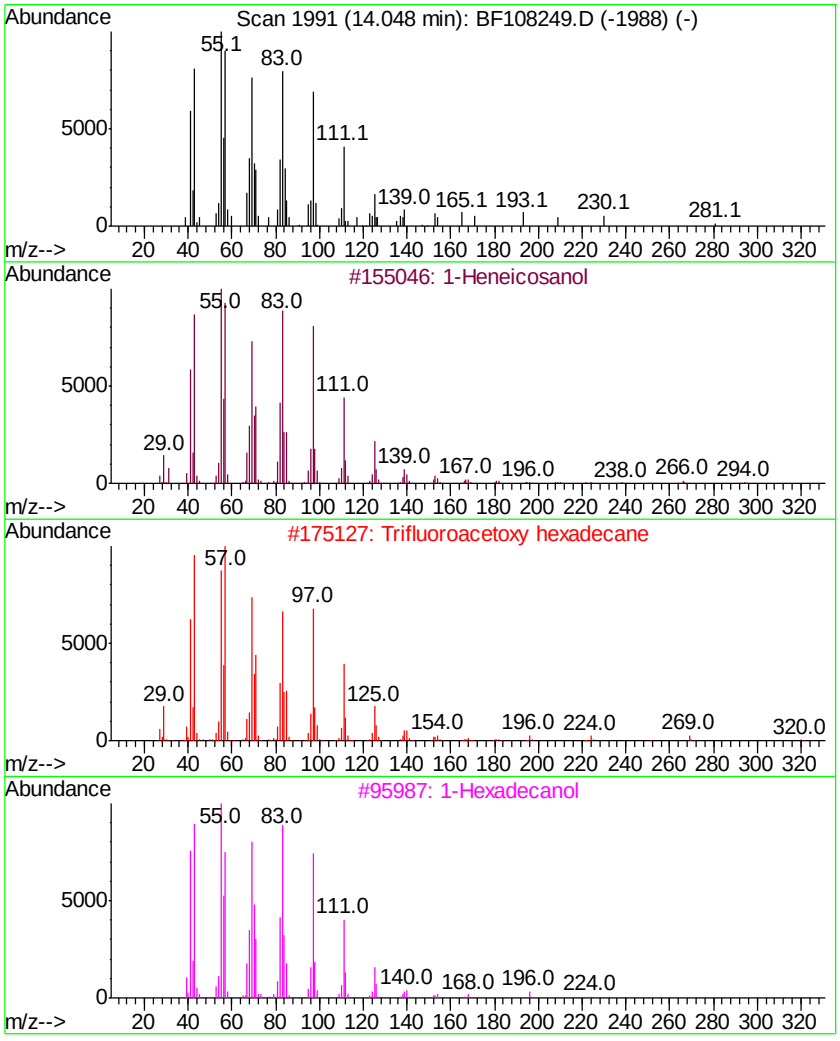
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

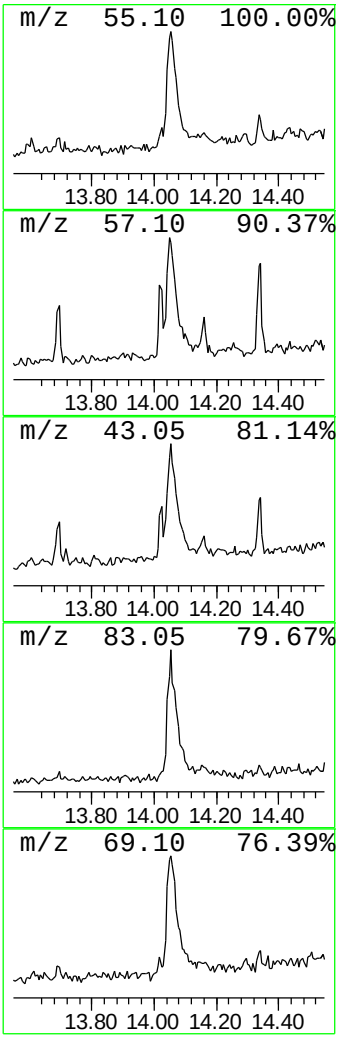
****

Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	2.97 ng	180961	Chrysene-d12	14.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	86
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	86
3	1-Hexadecanol	242	C16H34O	036653-82-4	62
4	Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	58
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
Data File : BF108249.D
Acq On : 17 Aug 2018 17:59
Operator : JU/SJ
Sample : J4500-21
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROCK

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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...	5.25	14.9	ng	648737	1	7.01	868764	20.0
unknown6.78	6.78	67.0	ng	2909300	1	7.01	868764	20.0
1-Heneicosanol	14.05	3.0	ng	180961	5	14.21	1217980	20.0